A COMPARATIVE STUDY OF VARIANT TURBULENCE MODELING IN THE PHYSICAL BEHAVIORS OF DIESEL SPRAY COMBUSTION

by

Behnaz AMINI * , Hasan KHALEGHI
Department of Mechanical Engineering, Tarbiat Modares University, Tehran, Iran

In this research, the performance of non-linear k-ε turbulence model in resolving the time delay between mean flow changes and its proportionate turbulent dissipation rate adjustment was investigated. For this purpose, the ability of Launder-Spalding linear, Suga non-linear, Yakhot RNG and Rietz modified RNG k-ε models are compared in the estimation of axial mean velocity profile and turbulent integral length scale evolution during engine compression stroke. Computed results showed that even though all the models can predict the acceptable results for velocity profile, for turbulent integral length scale curve, non-linear model is in a good agreement with modified RNG model prediction that depicts correspondence with experimental reported data, while other models show a different unrealistic behaviors. Also after combustion starts and piston is expanding, non-linear model can predicts actual manner for integral length scale while linear one cannot. It is concluded that, physical behavior of turbulence models characteristics should be ascertained before being successfully applied to simulate complex flow fields like internal combustion engines.

Key words: ***variant k-ε turbulence models, Partially Stirred Reactor combustion modeling, Non-linear k-ε turbulence, integral length scale, physical behaviors, engine flow***

1. INTRODUCTION

In recent years special attention has been paid to the topic of engine flow as one of the major researches, due to the fact that it involves the most complex aspects of turbulence, unsteady and highly compressible due to very large variations in combustion chamber volume, non-homogeneous multi-phase flows. These problems are tightly coupled and highly non-linear. In-cylinder, flow characteristics can greatly affect most of engine flow mechanisms such as fuel spray penetration, evaporation and distribution in combustion chamber, flame ignition and propagation, heat transfer and even turbulent eddies. As a result improper modeling of in-cylinder flow characteristics may give a poor estimation of engine flow mechanisms so choosing a proper method for simulating both turbulence and chemistry is important.

Even though, the Launder-Spalding linear two-equation k-ε model [1], employing Boussinesq approximation, have been successfully tested in a wide variety of steady state flows occurring in technical applications, they are not expected to present satisfactory results in calculating engine turbulent flow characteristics and consequently the engine flow mechanisms discussed earlier owing to they have been developed for incompressible and stationary flows. In order to compensate the weaknesses of linear k-ε models various approaches have been investigated by researchers during these years.

* Corresponding author; e-mail: behnaz.aminii@gmail.com

For the non-linear k-ε model that was introduced by Speziale [2] and developed by Suga [3], the Boussinesq approximation is used to develop a relation between turbulent stress and strain rate tensors which is a function of strain and vorticity tensors. This model was used for modeling turbulence phenomena by Behzadi et al. [4] in KIVA base code.

Based on the theory of re-normalization groups, the RNG k-ε model was developed by Yakhot et al. [5] and successfully incorporated to spray combustion modeling by Han et al. [6] as a further development of a study by Coleman and Mansour [7]. Considering the important role of compressibility in turbulent structures of engine flows, researches have been focused on developing compressible turbulence models recently. Default choice of most engine flow computational codes is the modified version of Launder-Spalding k-ε model which was corrected to account for compressibility effects by Tahry [8]. Coleman et al. introduced an additional closure relation to account for engine flow rapid distortions [7].

Rietz et al. proposed a correction for turbulence dissipation rate of the RNG k-ε model based on non-equilibrium turbulence considerations from the rapid distortion theory. According to this method, there is always a time delay between mean flow rapid changes and its proportionate turbulent dissipation rate adjustment [9].

The turbulence – chemistry interaction is very strong and it is therefore essential to have a reliable interaction model for this process if accurate predictions of emissions are to be performed. To account for the influence of the turbulent fluctuations on the reaction rate the Partially Stirred Reactor (PaSR) approach has been used. PaSR concept by Karlsson [10] in 1995 is an extension of the Eddy Break Up (EBU) approach. It was further developed by Golovitch [11] in 2000. This model was used for calculating the turbulence – chemistry by Nordin [12] in 2001 in KIVA 3-V code.

2. MATERIAL AND METHODS

2.1. A brief introduction to computational code

In this research, above mentioned turbulence models will be introduced to a PISO algorithm-based code in order to compute in-cylinder axi-symmetric flow calculations. Droplet evaporations, breakup and collisions are also modeled in this computational code. Evaporation will be calculated by Bornman and Johnson equations. Collision calculations are based on the O'Rourke and Bracco models. Droplets turbulent dispersion phenomenon will be taken into account using random walk method too. Previous studies show significant correspondence between the results of this code and results of well-known engine codes and also experiments [13, 14]. Although spray and air-fuel mixing will not be directly dealt with in the present study, the performance of this numerical code will be examined in engine two- phase flow as well. Therefore, air and fuel mixing models will be reviewed briefly here in after. Numerical modeling of air and fuel mixing was developed by Jones and Watkins for reciprocating engines based on local homogeneous flow assumptions and spray calculations were supposed to be a "separated flow" type [15-17]. This code in fact employs a Lagrangian-Eulerian approach utilizing finite volume discretization method. Two-phase flow calculations are also done by random parcels method which is a version of discrete droplet model regarding stochastic considerations.

2.2. Flow calculations domain

The capability of the four turbulence models discussed above will be investigated in control and resolving the time delay between mean flow changes and turbulence dissipation rate adjustment in a flat piston diesel engine with a 30×30 grid. The geometrical parameters and specifications of the computational domain have been depicted in fig. 1 and tab. 1, respectively.

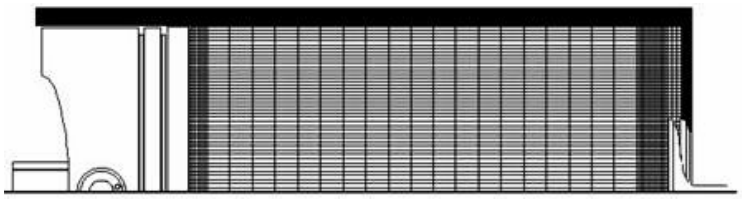

Figure 1. Geometry and grid lines at 180° crank angle

Table 1. Specifications of the computational domain

Bore (mm)	75
Stroke (mm)	94
Compression Ratio	10.5
Engine speed (rpm)	3000
Valve radius (mm)	17
Max. opening of valve (mm)	7.3

3. MATHEMATICAL MODEL

3.1. Droplet Phase Equations

As mentioned above, the spray is simulated by a number of computational parcels, all containing a different number of representative droplets with identical properties. These parcels are tracked in time and space as they traverse the gas field by solving the following basic equations for a single droplet:

3.1.1. Droplets Trajectory Equation

Axial and radial droplets trajectory equations respectively can be expressed as eq. (1) and eq. (2)

$$u_d = \frac{dx_d}{dt} \tag{1}$$

$$v_d = \frac{dr_d}{dt} \tag{2}$$

3.1.2.Equation of Motion of Droplets

Eq. (3) and eq. (4) are axial momentum and radial momentum of droplets

$$\frac{du_d}{dt} = \frac{3}{4} C_D \frac{\rho_g}{\rho_d} \frac{V_{rel}}{D_d} (u + u' - u_d) - \frac{1}{\rho_g} \frac{dp}{dx} \tag{3}$$

$$\frac{dv_d}{dt} = \frac{3}{4} C_D \frac{\rho_g}{\rho_d} \frac{V_{rel}}{D_d} (v + v' - v_d) - \frac{1}{\rho_g} \frac{dp}{dr} \tag{4}$$

In which V_{rel} is the relative velocity of two phases can be expressed as eq. (5)

$$V_{rel} = [[(u + u') - u_d]^2 + [(v + v') - v_d]^2]^{0.5} \tag{5}$$

3.1.3. Droplets Mass Conservation Equation

The evaporation rate is expressed in terms of mass, or diameter and rate of evaporation for a single droplet is given by the expression,

$$\frac{dm_d}{dt} = -\pi D_d D P_t \ln\{(P_t - P_{v,\infty})/(P_t - P_{v,s})\} Sh / RT_m \tag{6}$$

3.1.4. Droplets Energy Conservation Equation

The liquid droplet receives its energy from the gas, which is used to increase the liquid temperature and overcome the latent heat of evaporation in order to evaporate the fuel. The evaporation process will receive its energy from droplet.

$$\frac{d(mc_pT)_d}{dt} = \pi D_d K (T_g - T_d) \{Z/(e^z - 1)\} Nu + Q \frac{dm_d}{dt} \tag{7}$$

$$Z = -\frac{C_{pv} \frac{dm_d}{dt}}{\pi D_d K Nu} \tag{8}$$

3.2. Gas Phase Equations

The analysis of the gas phase involves solving equations for mass, momentum and energy together with the fuel vapor mass fraction and species concentration. Included are also the turbulence kinetic energy and dissipation rate for the gas phase turbulence. In addition to the conventional single-phase flow analysis, a droplet phase source term $S_{\phi d}$ must be added to conservative equations which represent the influences of converted mass from droplets phase to gas phase in unit second. Effects of void fraction θ, the ratio of occupied volume by gas phase, on the governing equations must also be considered for dense sprays. The governing equations for the gas phase can be expressed as a general transport equation, eq. (9):

$$\frac{\partial(\rho\theta\phi)}{\partial t}+\frac{\partial(\rho\theta u\phi)}{\partial x}+\frac{1}{r}\frac{\partial}{\partial r}(r\rho\theta v\phi)=\frac{\partial}{\partial x}(\Gamma\theta\frac{\partial\phi}{\partial x})+\frac{1}{r}\frac{\partial}{\partial r}(\Gamma r\theta\frac{\partial\phi}{\partial r})+\theta S_{\phi}+S_{\phi d} \qquad (9)$$

With using linear k-ε turbulence model, tab. 2 illustrates S_{ϕ} , this amount will be changed when other k-ε turbulence models is used, tab. 3 depicts the droplet phase source term $S_{\phi d}$ that must be added to conservative equations.

Table 2. Source terms

Conservation Eq.	ϕ	Γ	S_{ϕ}
Mass	1	0	0
Axial Momentum	u	μ_{eff}	$-\frac{\partial p}{\partial x}+(\frac{\partial}{\partial x}(\mu_t\frac{\partial u}{\partial x})+\frac{1}{r}\frac{\partial}{\partial r}(r\mu_t\frac{\partial v}{\partial x})-\frac{2}{3}\frac{\partial}{\partial x}(\mu_t\nabla.u+\rho k)$
Radial Momentum	v	μ_{eff}	$-\frac{\partial p}{\partial r}+\frac{\partial}{\partial x}(\mu_t\theta\frac{\partial u}{\partial r})+\frac{1}{r}\frac{\partial}{\partial r}(r\mu_t\theta\frac{\partial v}{\partial r})-\frac{2}{3}\frac{\partial}{\partial x}[\mu_t\theta\nabla.U+\rho\theta k]-2\mu_t\theta\frac{v}{2}$
Species Vapor Mass Fraction	Y_i	$\frac{\mu}{\sigma_Y}$	$K\dot{\omega}_i$
Energy	h	$\frac{\mu}{\sigma_h}$	$K\dot{\omega}_h$

K is extracted from the Partially Stirred Reactor (PaSR) model that is described in detail in section 5 , and effective viscosity is expressed as eq. (10),

$$\mu_{eff}=\mu+\mu_t \qquad (10)$$

Table 3. Droplet phase source term $S_{\phi d}$

Conservation Eq.	$S_{\phi d}$
Mass	$S_{md}=-\frac{\pi}{6}\frac{\rho_d}{\delta t}\sum_k N_{d,k}[(D_{d,k}^{n+1})^3-(D_{d,k}^{n})^3]$
Axial Momentum	$S_{ud}=-\frac{\pi}{6}\frac{\rho_d}{\delta t}\sum_k N_{d,k}[(D_{d,k}^{n+1})^3U_{d,k}^{n+1}-(D_{d,k}^{n})^3U_{d,k}^{n}]$
Radial Momentum	$S_{vd}=-\frac{\pi}{6}\frac{\rho_d}{\delta t}\sum_k N_{d,k}[(D_{d,k}^{n+1})^3V_{d,k}^{n+1}-(D_{d,k}^{n})^3V_{d,k}^{n}$
Fuel vapor mass fraction	$S_{md}=-\frac{\pi}{6}\frac{\rho_d}{\delta t}\sum_k N_{d,k}[(D_{d,k}^{n+1})^3-(D_{d,k}^{n})^3]$
Energy	$S_{hd}=-\frac{\pi}{6}\frac{\rho_d}{\delta t}\sum_k N_{d,k}[(D_{d,k}^{n+1})^3(C_pT_{d,k})^{n+1}-(D_{d,k}^{n})^3(C_pT_{d,k})^{n}]$

3.3. Turbulent flow modeling

Equations of the k-ε model, turbulence kinetic energy and turbulent dissipation rate, are expressed respectively as eq. (11), eq. (12)

$$\frac{\partial}{\partial t}(\rho\theta k)+\frac{\partial}{\partial x}(\rho\theta uk)+\frac{1}{r}\frac{\partial}{\partial r}(r\rho\theta vk)=\frac{\partial}{\partial x}(\frac{\mu_t}{\sigma_k}\theta\frac{\partial k}{\partial x})+\frac{1}{r}\frac{\partial}{\partial r}(\frac{\mu_t}{\sigma_k}\theta r\frac{\partial k}{\partial r})]+\theta S_k \tag{11}$$

$$\frac{\partial}{\partial t}(\rho\theta\varepsilon)+\frac{\partial}{\partial x}(\rho\theta u\varepsilon)+\frac{1}{r}\frac{\partial}{\partial r}(r\rho\theta v\varepsilon)=\frac{\partial}{\partial x}(\frac{\mu_t}{\sigma_\varepsilon}\theta\frac{\partial\varepsilon}{\partial x})+\frac{1}{r}\frac{\partial}{\partial r}(\frac{\mu_t}{\sigma_\varepsilon}\theta r\frac{\partial\varepsilon}{\partial r})+\theta S\varepsilon \tag{12}$$

3.3.1. Linear k-ε turbulence model

For Linear model Boussinesq approximation and turbulence viscosity are expressed as eq. (13) and eq. (14):

$$-\rho\overline{u_i'u_j'}=\mu_t(S_{ij}-\frac{1}{3}S_{kk}\delta_{ij})-\frac{2}{3}\rho k\delta_{ij} \tag{13}$$

$$\mu_t=C_\mu\rho\frac{k^2}{\varepsilon} \tag{14}$$

Equations of k-ε model, turbulence kinetic energy and turbulent dissipation rate, are expressed respectively as eq. (15) and eq. (16):

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x}(\rho uk)+\frac{1}{r}\frac{\partial}{\partial r}(r\rho vk)=\frac{\partial}{\partial x}(\frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial x})+\frac{1}{r}\frac{\partial}{\partial r}(\frac{\mu_t}{\sigma_k}r\frac{\partial k}{\partial r})]+(P_k-\rho\varepsilon) \tag{15}$$

$$\begin{aligned}&\frac{\partial}{\partial t}(\rho\varepsilon)+\frac{\partial}{\partial x}(\rho u\varepsilon)+\frac{1}{r}\frac{\partial}{\partial r}(r\rho v\varepsilon)=\frac{\partial}{\partial x}(\frac{\mu_t}{\sigma_\varepsilon}\frac{\partial\varepsilon}{\partial x})+\frac{1}{r}\frac{\partial}{\partial r}(\frac{\mu_t}{\sigma_\varepsilon}r\frac{\partial\varepsilon}{\partial r})+\\&(\frac{\varepsilon}{k}(C_{\varepsilon1}P_k-C_{\varepsilon2}\rho\varepsilon)+C_{\varepsilon3}\rho\varepsilon\nabla.U)\end{aligned} \tag{16}$$

In which,

$$P_k=-\rho\overline{u_i'u_j'}\frac{\partial u_i}{\partial x_j} \tag{17}$$

Constant coefficient of linear k-ε turbulence model are given in tab. 4

Table 4. Linear k-ε turbulence model constant

$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	$C_{\varepsilon 3}$	σ_k	σ_ε	C_μ
1.44	1.92	-1.0	1.0	1.3	0.09

3.3.2. Non-linear k-ε turbulence model

For the Suga non-linear model the Boussinesq approximation is used to develop a relation, between turbulent stress and strain rate tensors which is a function of strain and vorticity tensors. The Boussinesq approximation for second order non-linear model has quadratic products of the strain and vorticity tensor to improve the prediction of secondary flows involving the normal stress effects.

$$-\rho\overline{u_i'u_j'} = \mu_t(S_{ij} - \frac{1}{3}S_{kk}\delta_{ij}) - \frac{2}{3}\rho k\delta_{ij} - C_1\frac{\mu_t k}{\varepsilon}(S_{ik}S_{kj} - \frac{1}{3}S_{kl}S_{kl}\delta_{ij}) \\ -C_2\frac{\mu_t k}{\varepsilon}(\Omega_{ik}S_{kj} + \Omega_{jk}S_{ki}) - C_3\frac{\mu_t k}{\varepsilon}(\Omega_{ik}\Omega_{jk} - \frac{1}{3}\Omega_{kl}\Omega_{kl}\delta_{ij}) \tag{18}$$

In addition, for third order non-linear model, with adding the cubic terms to Boussinesq approximation it can lead to better results in modeling of flows with streamline curvature, as claimed in [4].

$$-\rho\overline{u_i'u_j'} = \mu_t(S_{ij} - \frac{1}{3}S_{kk}\delta_{ij}) - \frac{2}{3}\rho k\delta_{ij} - C_1\frac{\mu_t k}{\varepsilon}(S_{ik}S_{kj} - \frac{1}{3}S_{kl}S_{kl}\delta_{ij}) - C_2\frac{\mu_t k}{\varepsilon}(\Omega_{ik}S_{kj} + \Omega_{jk}S_{ki}) - \\ C_3\frac{\mu_t k}{\varepsilon}(\Omega_{ik}\Omega_{jk} - \frac{1}{3}\Omega_{kl}\Omega_{kl}\delta_{ij}) - C_4\frac{\mu_t k^2}{\varepsilon^2}(S_{ki}\Omega_{lj} + S_{kj}\Omega_{li})S_{kl} - C_5\frac{\mu_t k^2}{\varepsilon^2}(\Omega_{il}\Omega_{lm}S_{mj} + S_{il}\Omega_{lm}\Omega_{mj} - \frac{2}{3}S_{lm}\Omega_{mn}\Omega_{nl}\delta_{ij}) - \\ C_6\frac{\mu_t k^2}{\varepsilon^2}S_{kl}S_{kl}(S_{ij} - \frac{1}{3}S_{kk}\delta_{ij}) - C_7\frac{\mu_t k^2}{\varepsilon^2}\Omega_{kl}\Omega_{kl}(S_{ij} - \frac{1}{3}S_{kk}\delta_{ij}) \tag{19}$$

In which,

$$S_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \tag{20}$$

$$\Omega_{ij} = \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \tag{21}$$

Unlike linear model, for calculating turbulence viscosity, C_μ is not constant and it is a function of strain and vorticity tensors to assist the sensitivity of the model to stream line curvature:

$$C_{\mu} = \frac{0.3}{1+0.35(\max(\widetilde{S},\widetilde{\Omega}))^{1.5}}(1-EXP[\frac{-0.36}{EXP(-0.75\max(\widetilde{S},\widetilde{\Omega}))}]) \tag{22}$$

Where the non-dimensional strain, $\widetilde{S}$, and vorticity, $\widetilde{\Omega}$ are defined as eq. (23) , eq. (24):

$$\widetilde{S} = \frac{k}{\varepsilon}\sqrt{0.5S_{ij}S_{ij}} \tag{23}$$

$$\widetilde{\Omega} = \frac{k}{\varepsilon}\sqrt{0.5\Omega_{ij}\Omega_{ij}} \tag{24}$$

as claimed in [3].

Constant coefficient of Suga non-linear k-ε turbulence model are given in tab. 5,

Table 5. Suga non-linear k-ε turbulence model constants

C_1	C_2	C_3	C_4	C_5	C_6	C_7
-0.1	0.1	0.26	$-10c_{\mu}{}^2$	0.0	$-5c_{\mu}{}^2$	$5c_{\mu}{}^2$

3.3.3. RNG k-ε turbulence model

The RNG k-ε model was developed to account for the effects of smaller scales of motion in the standard k-ε model. For this purpose, Yakhot et al. suggested the inclusion of an extra term in right-hand side of the turbulence dissipation rate equation of the standard k-ε model. This term (R) is of the same order of magnitude as the standard ε-production term in the flow regions of large strain rate (e.g. recirculating flows or flows undergoing strong compression) and therefore can correct its value. In this model turbulence kinetic energy is expressed as eq. (25),

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x}(\rho u k)+\frac{1}{r}\frac{\partial}{\partial r}(r\rho v k)=\frac{\partial}{\partial x}((\mu+\frac{\mu_t}{\sigma_k})\frac{\partial k}{\partial x})+\frac{1}{r}\frac{\partial}{\partial r}((\mu+\frac{\mu_t}{\sigma_k})r\frac{\partial k}{\partial r})]+(P-\rho\varepsilon) \tag{25}$$

Also turbulent dissipation rate is expressed as eq. (26),

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\frac{\partial}{\partial x}(\rho u\varepsilon)+\frac{1}{r}\frac{\partial}{\partial r}(r\rho v\varepsilon)=\frac{\partial}{\partial x}((\mu+\frac{\mu_t}{\sigma_\varepsilon})\frac{\partial\varepsilon}{\partial x})+\frac{1}{r}\frac{\partial}{\partial r}((\mu+\frac{\mu_t}{\sigma_\varepsilon})r\frac{\partial\varepsilon}{\partial r})+(C_{\varepsilon 1}\frac{\varepsilon}{k}P-C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k}+R) \tag{26}$$

Turbulence viscosity is expressed as eq. (14). In eq. (25) and eq. (26) P is turbulence energy production and will be found from the following relation:

$$P=\mu_t(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i})\frac{\partial u_i}{\partial x_j} \tag{27}$$

R ,the last term of dissipation rate, will be formulated as:

$$R=-\frac{\rho C_\mu\eta^3(1-\frac{\eta}{\eta_0})\varepsilon^2}{(1+\beta\eta^3)k} \tag{28}$$

In which,

$$\eta=\frac{Sk}{\varepsilon} \tag{29}$$

$$S_{ij}=\frac{1}{2}(\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}) \tag{29}$$

$$S^2=2S_{ij}S_{ij} \tag{30}$$

Constant coefficient of RNG k-ε Turbulence Model are given in tab. 6,

Table 6.RNG turbulence model constants

σ_k	σ_ε	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	β	η_0	C_μ
0.72	0.72	1.42	1.68	0.015	4.38	0.085

3.3.4. Rietz modified RNG turbulence model

Rietz modified RNG turbulence model was introduced in order to obtain a physical behavior for turbulent characteristics of engine flow. Rietz et al. proposed a correction to the term of turbulence dissipation rate. Non-equilibrium turbulence considerations from rapid distortion theory have been utilized to derive a correction to the turbulence dissipation rate [9],

$$\varepsilon \propto \frac{\varepsilon_{eq}}{\mathrm{Re}_t} \tag{32}$$

In which

$$\mathrm{Re}_t \propto \frac{\nu_t}{\nu} \tag{33}$$

4. THE PARTIALLY STIRRED REACTOR MODEL

Under high-intensity conditions, turbulence exerts the main influence on the mechanism of turbulence combustion. Due to the thinness and complex structure of the flame, the computation cell size has to be several orders of magnitude larger than required to resolve the flame structure. It is still not possible, with current computer technology, to resolve the flame structure for practical purposes. Since it is only possible to resolve variables, e.g., species concentrations, on a scale which is of the same order as the cell size, the conditions in the combustion zone are thus, in principle, unknown. The Partially Stirred Reactor (PaSR) model has been generalized to account for the effect of mixture imperfections.

In PaSR approach, a computational cell is split into two different zones, one zone, in which all reactions occur, and another, in which no reactions occur. Thus, the composition changes due to mass exchange with the reacting zone. Furthermore, the reacting zone is treated as a perfectly stirred reactor (PSR), in which the composition is homogeneous (every species is assumed to be perfectly mixed with the other ones). This allows us to disregard any fluctuations when calculating the chemical source terms. The reactive mass fraction will be defined below as the calculation is advanced one time step, from C_0 to C_1. Fig 2 shows the conceptual picture of PaSR model.

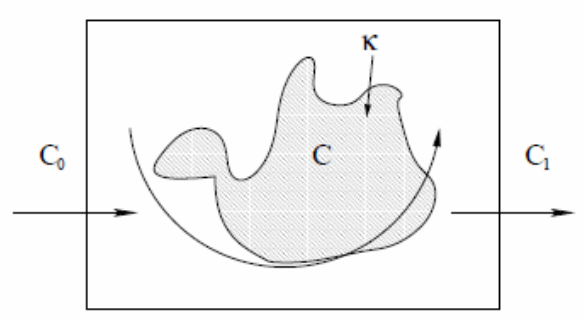

Figure 2. Conceptual Picture of a PaSR

C_0 is the averaged concentration in the feed of the cell and may be considered as the initial averaged concentration in cell, C is the unknown concentration in the reaction zone, C_1 is the time averaged reactor-exit concentration. This is also the averaged concentration in cell,

$$C_1 = KC + (1-K)C_0 \tag{34}$$

Where K is the mass fraction of the mixture that reacts. To estimate this fraction, it seems quite clear that it shall be proportional to the ratio of chemical reaction time τ_{ch} to the total conversion time in the reactor that it is the sum of the micro-mixing time τ_{mix} and reaction time τ_{ch}.

$$K = \frac{\tau_{ch}}{\tau_{ch} + \tau_{mix}} \tag{35}$$

τ_{mix} from Taylor time scale, is expressed as:

$$\tau_{mix} = C_{mix}\frac{k}{\varepsilon} \tag{36}$$

C_{mix} is a constant between 0.001 and 0.3.
τ_{ch} is expressed as:

$$\frac{1}{\tau_{ch}} = \frac{\dot{\omega}_h}{\Delta H_{combustion}} \tag{37}$$

Consider the following reaction:

$$\sum_{i=1}^{N} \alpha_{ij}^{+} f_i \underset{k_j^-}{\overset{k_j^+}{\rightleftharpoons}} \sum_{i=1}^{N} \alpha_{ij}^{-} f_i \tag{38}$$

The rate equation for eq. (38) is:

$$RR_j^{\pm} = k_j^{\pm} \prod_{i=1}^{N} [f_i]^{\alpha_{ij}^{\pm}} \tag{39}$$

For finding the combustion terms of source term S_ϕ in eq. (9) for species vapor mass fraction and energy equations eq. (40) and eq. (41) must be used.

$$\dot{\omega}_i = \sum_{j=1}^{R} (\alpha_{ij}^{-} - \alpha_{ij}^{+})(RR_j^{+} - RR_j^{-}) \tag{40}$$

$$\dot{\omega}_h = \sum_{j=1}^{R} (-\Delta H_j)(RR_j^+ - RR_j^-) \tag{41}$$

$$\Delta H_j = \sum_{i=1}^{N} (\alpha_{ij}^+ - \alpha_{ij}^-)(h_i)_f^{ref} \tag{42}$$

$(h_i)_f$ is standard heat of formation of a species, eq. (41) also is used in eq. (37).

$$\Delta H_{combustion} = \sum_{j=1}^{R} \Delta H_j \tag{43}$$

5. VALIDATION OF THE MODEL AND CALCULATIONS

Generally, a preliminary work is required to ensure that the numerical solutions are independent of mesh size and the time step. So, in order to examine the sensitivity of calculated results to grid size and time step, flow field was solved with three different mesh sizes of 30×30, 40×40 and 45×45. The Time step independency of results was also investigated with five equivalent time steps of 1, 0.75, 0.5, 0.25 and 0.125 degree of crank angle (namely, 55.5, 41.6, 27.8, 13.9, 6.9 microseconds respectively). Computed results demonstrated that a 30×30 grid and an equivalent time step of 0.125 degree of crank angle (6.9 microseconds) present a grid and time independent solution. In order to evaluate the computational code, axial mean velocity profile calculated with Suga non-linear and RNG k-ε turbulence models compared with its experimental data reported in [14] in a cross section of a flat head piston at 15mm distance from the cylinder head, the specification of which is listed in tab.1, at 90° crank angle . As shown in fig. 3, calculated velocity profiles are correspondent with the one obtained from experiment.

Evaluation of the present numerical code will be fulfilled if such a comparison between numerical and experimental data is carried out in the case of in-cylinder two-phase flow when the fuel is injected into the combustion chamber. Spray tip penetration length into the combustion chamber is an important parameter in spray structure and has a great role in performance of internal combustion engines. Therefore, in this section the spray tip penetration length computed with non-linear turbulence model was compared with experimental data reported in [18] in which the initial combustion chamber pressure and temperature conditions were set to be 20 bar and 300 K respectively. As seen in fig. 4, Suga non-linear turbulence model calculations show a high degree of correspondence with experimental reported data.

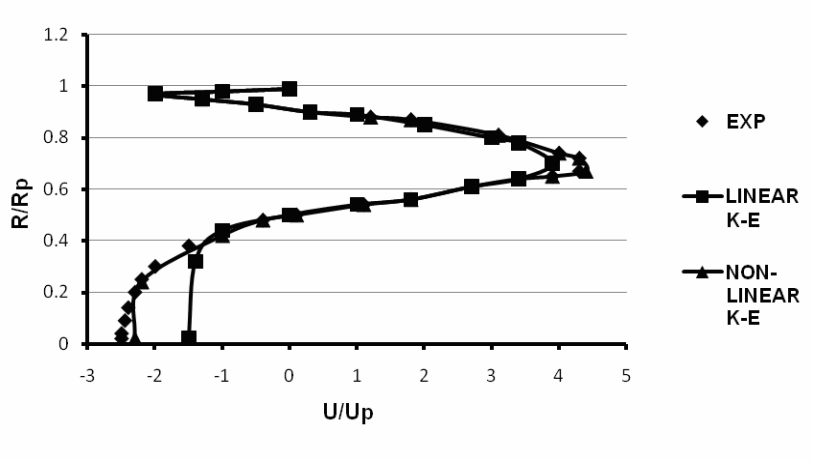

Figure 3. Compartion of calculated axial mean velocity profile with experimental result

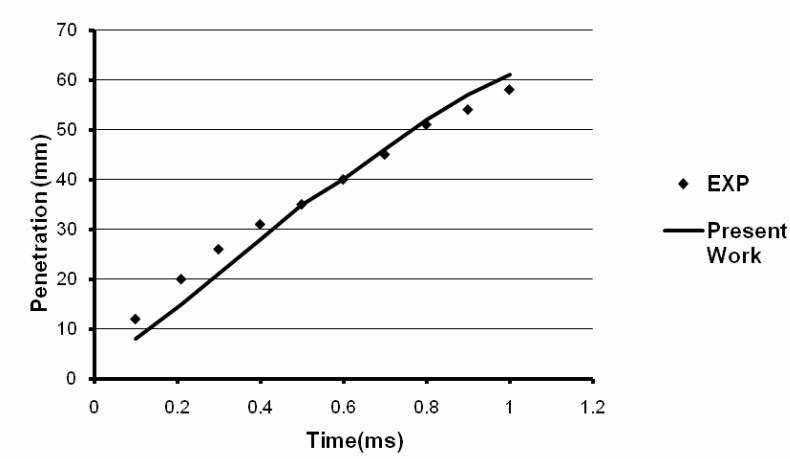

Figure 4. Compartion of calculated spray penetration length with expremental result

6. RESULT AND DISCUSSION

The objective of this study is a Comparative assessment of variant k-ε models for engine flow applications and implementation of Non-linear k-ε turbulence model in-cylinder flow and assessing its capability in resolving the time delay between mean flow rapid changes and its proportionate eddy dissipation adjustment. According to the fact that the flow field will experience a continuous reduction in volume during compression stroke, integral length scale which delivers a description of flow field overall size is also expected to decrease [9]. Integral length scale can be computed from the following relation:

$$L_I = C_\mu \frac{k^{1.5}}{\varepsilon} \tag{44}$$

The behavior of the turbulent integral length scales are presented in fig. 5.

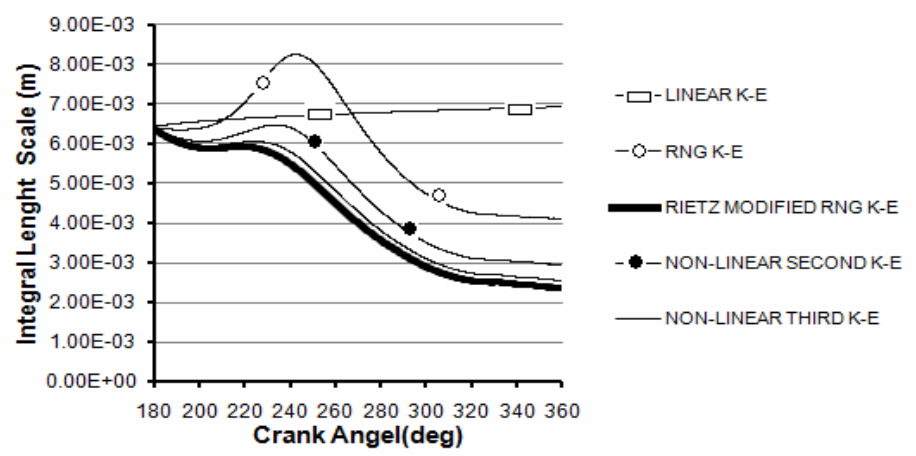

Figure 5. Compartion of integral length scale with using variant k-ε models

Linear k-ε depicts a gradual continuous increment as the combustion chamber compresses to top dead center, so this result accounts for not only this model is not realistic, but also it is not sensitive enough to variation of flow field volume, this model gives a quite poor estimation of time delay between mean flow rapid changes and adjustment in small dissipative scales of the flow during compression stroke. Although first the RNG model reveals an increment in integral length scale which is not physical while the combustion chamber compresses, near the top dead center the trend becomes acceptable. According to [9] the Rietz modified RNG turbulence model has been validated with experimental data. As it can be seen Suga non-linear second order k-ε turbulence model presents near results to Rietz modified RNG but still demonstrates an upward trend until crank angle 240. Suga non-linear third order k-ε turbulence model has a very good agreement with the Rietz modified RNG.

Fig. 6 illustrates the integral length scale after combustion starts, at crank angle 358, for linear and non-linear k-ε turbulence models.

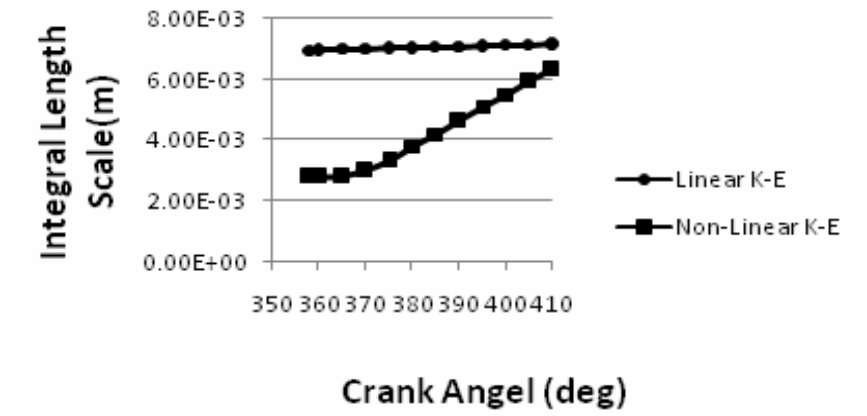

Figure 6. Compartion of integral length scale during combustion stroke

Since piston is expanding rapidly in the late compression phase, the cylinder volume is increasing and integral length scale is increasing accordingly [9]. This behavior is well reflected by the non-linear model.

In contrast, the linear k-ε computation account for an almost constant integral length scale during this expansion phase, which is inconsistent with the increasing cylinder volume determining the squish flow.

7. CONCLUSION

Taking every proofs into consideration it can be concluded that, although in some features like the axial mean velocity profile, illustrated in fig. 2, all the models can predict the acceptable results, for integral length scale solely modified RNG and non-linear third order models depict correspondence with experimental reported data [9]. Physical behaviors of turbulence models characteristics should be ascertained before being successfully applied to simulate complex flow fields like internal combustion engines.

NOMENCLATURE

C □ Concentration, [mol/m^3]
C_D □ Drag Coefficient, [□]
C_p □ Specific heat, [J kg^{-1}K^{-1}]
D_d □ Droplet diameter, [m]
D □ Mass diffusion coefficient, [m^2 s^{-1}]
h □ Gas enthalpy, [J kg^{-1}]
K □ Thermal conductivity, [W m^{-1} K^{-1}]
k □Turbulent kinetic energy, [m^2 s^{-2}]
P_t □Total pressure, [Pa]
$P_{v,\infty}$ □ Vapor pressure away from droplet surface, [Pa]
$P_{v,s}$ □ Vapor pressure at droplet surface, [Pa]
Q □ Latent heat, [J kg^{-1}]
R □ Gas constant, [J mol^{-1} K^{-1}]
S □ Strain tensor, [s^{-1}]
$\tilde{S}$ □ Non-dimensional strain, [□]
T_m □ mean temperature, [$^\circ K$]
T □ Temperature, [$^\circ K$]
u □ Axial velocity, [ms^{-1}]
v □ Radial velocity, [ms^{-1}]
ρ □ Density, [kg m^{-3}]
ε □ Turbulent dissipation rate ,[m^{2}s^{-3}]
ε_{eq} □ Equilibrium turbulence ,[m^{2}s^{-3}]
Ω □Vorticity tensor, [s^{-1}]
$\tilde{\Omega}$ □ Non-dimensional vorticity, [□]
μ_t □ Turbulence viscosity, [Pa s]
ν □ Molecular (Kinematic) viscosity, [m^2 s^{-1}]
ν_t □ Turbulent viscosity, [m^2 s^{-1}]
Nu □ Nusselt number (=$(\rho v D_d/\mu)^{0.5}\times(\mu C_p/k)^{0.33}$),[□]
Sh □Sherwood number (=$(\rho v D_d/\mu)^{0.5}\times(\mu/\rho D_d)^{0.33}$),[□]
Re_t □Turbulence Reynolds number
σ_t □ Prandtl number for turbulent flow
$N_{d,k}$ □ Number of droplets in each parcel
δt □ Interval between two continuous time
τ □ time

Subscripts
$_d$ □ Related to droplet
$_g$ □ related to gas phase

Superscript
$(')$ □ indicates gas phase velocity components fluctuations

REFERENCES

[1] Launder, B. and D. Spalding, The numerical computation of turbulent flows, Comp methods in app. mech and eng 3, 1974.
[2] C.G. Speziale, On Non-linear $k-l$ and $k-\varepsilon$ Models of Turbulence, Fluid Mechanics journal vol 178, 1987 .
[3] K.Suga, Development and Application of a cubic Eddy-Viscosity Model of Turbulence, Int . J.Heat and Fluid Flow,Vol.17 No 2,1996.
[4] S.A.Behzadi,A.P.Watkins, Flow and Turbulence Modeling in a Motored Reciprocating Engine using a Cubic Non-linear Turbulence Model, 4th International Symposium on Engineering Turbulence Modeling,1999.
[5] V. Yakhot and L. M. Smith, The renormalization group, the ε- expansion and derivation of turbulence models. J. Sci. Comp., 7:35-61, 1992.

[6] Z.Y. Han and R.D. Reitz, Turbulence modeling of internal combustion engines using RNG $k-\varepsilon$ models, Combust. Sci. and Tech., 106:267-295, 1995.

[7] G.N. Coleman and N.N. Mansour, Modeling the Rapid Spherical Compression of Isotropic Turbulence, Physics of Fluids A, Vol. 3 No. 9, 1991.

[8] S.H. El Tahry, $k-\varepsilon$ Equations for Compressible Reciprocating Engine Flows, AIAA Journal of Energy, Vol. 7 No. 4, 1983.

[9] F. Tanner, G. Zhu and R. Reitz, A Turbulence Dissipation Correction to the k-epsilon Model and Its Effect on Turbulence Length Scales in Engine Flow, International Multidimensional Engine Modeling Users Group Meeting at the SAE Congress, Detroit, 2001.

[10] Karlsson, J.A.J,:Modeling Auto-Ignition, Flame Propagation and Combustion in Non-Stationary Turbulent Sprays. In: PhD Thesis, Chalmers University of Technology, Goteborg,(1995)

[11] Golovitch,V.I,: Revising Old Good Models, Magnussen Eddy Dissipation Concept. In: Proceedings of Topical Meeting on Modeling of Combustion, Turku,Finnland,(2000)

[12] Nordin, P.A,'complex chemistry modeling of diesel spray combustion', PhD thesis, Chalmers university of technology,2001

[13] S.L. Yang, Y.K. Siow, C.Y. Teo and K. Hanjalic, A KIVA Code with Reynolds-Stress Model for Engine Flow Simulation, Energy, 30, 2005.

[14] Y. Khern Siow, A Reynolds-stress Turbulence Model in the KIVA Code for Engine Simulation, PhD Thesis, Michigan Technological University, 2003.

[15] M.M. El Wakil, O.A. Ueyhara and F.S. Myers, A Theoretical Investigation of the Heating-Up Period of Injected Fuel Droplets Vaporizing in Air, NACA Technical Note, 3179, 1954.

[16] M. Gavaises, Modeling of Diesel Fuel Injection Processes, PhD Thesis, Imperial College of Science and Technology and Medicine, University of London, London, 1997.

[17] A.D. Gossman and E. Ioannidies, Aspects of Computer Simulation of Liquid-Fuelled Combustors, Energy, 7 (6), 1983.

[18] M.A. Leschziner, Modeling Turbulent Recirculating Flows by Finite-Volume Methods-Current Status and Future Directions, International Journal of Heat and Fluid Flow, Vol. 10, No. 3, 1989