

# Large Eddy Simulation of Premixed Combustion in Spark Ignited Engines Using a Dynamic Flame Surface Density Model

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## ABSTRACT

In this work, cyclic combustion simulations of a spark ignition engine were performed using the Large Eddy Simulation techniques. The KIVA-4 RANS code was modified to incorporate the LES capability. The flame surface density approach was implemented to model the combustion process. Ignition and flame kernel models were also developed to simulate the early stage of flame propagation. A dynamic procedure was formulated where all model coefficients were locally evaluated using the resolved and test filtered flow properties during the fully developed phase of combustion. A test filtering technique was adopted to use in wall bounded systems. The developed methodology was then applied to simulate the combustion and associated unsteady effects in a spark ignition engine. The implementation was validated using the experimental data taken from the same engine.

Results show that, even with relatively coarser meshes used in this work, present LES implementation has been able to resolve the evolution of a large number of in-cylinder flow structures, which are more influential for engine performance. Predicted combustion rate and pressure rise is also in good agreement with the measurements. The limits of cyclic variations are well within the experimentally observed range. It has also been able to demonstrate the limits of cyclic fluctuations to a reasonable degree even with a fewer number of simulation cycles. A significant variation of flame propagation has also been predicted by the simulations.

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## INTRODUCTION

Use of the Large Eddy Simulation (LES) techniques has become increasingly popular for engineering simulations. In Reynolds Averaged Navier Stokes (RANS) method, the entire flow spectrum has to be modelled so that the predictions are model dependent to a larger extent. Whereas in LES, most of the flow field is resolved and only the sub-grid scale (SGS) part is modelled. Hence, LES results are more accurate, less model dependent and provide detailed information. In addition, LES is very much appropriate for engine simulations as it provides the opportunity to simulate inherent unsteady phenomena such as cyclic variations and combustion instabilities. Therefore, the use of LES in engine modelling provides a more reliable way of investigating operational and geometric refinements.

LES techniques have been widely used in non-reacting flow modelling, but its application to combustion simulation is still in a preliminary stage. In particular, studies devoted to internal combustion (IC) engine simulations using LES is very limited. Studies [1,2,3,4,5] may be identified as some of the promising cold flow simulations which reveal the

potential of LES predictions. Remarkably, compared to RANS, overall predictions of these simulations have found to be much better in agreement with experimental results. Application of LES in reacting flow modelling has largely been limited to non-premixed combustion [6, 7].

Premixed combustion modelling with LES is particularly a challenging task due to a number of difficulties detailed below. Usually, the premixed laminar flame thickness  $\delta_L$ , is so thin and it cannot be resolved using the classical LES mesh sizes. For example the flame thickness in SI engine applications is about 0.1 mm [8]. In order to adequately resolve the flame front, a minimum of 5-10 grid points are needed with a typical finite volume based CFD code [9]. Therefore, this resolution requirement is prohibitively expensive compared to the mesh resolution possible with current computing power, which is typically about 0.5mm.

A possible solution is to neglect this physical consideration and model the combustion process using an eddy break-up (EBU) type formulation. In such an approach, any modelling discrepancy may be absorbed by an adjustable model constant. The EBU model has two major short



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comings: negligence of the chemistry interaction with combustion and poor predictions near highly strained regions such as near walls. Moreover, the EBU model constant seems to be strongly dependent on the flow condition and mesh configuration. However, there is only very little work carried out to investigate the applicability of this type of formulations [10] and some initial applications of the LES-EBU model can be found in [11, 12].

The  $G$ -equation (level-set) approach is also an alternative method where the flame front is described as a zero thickness surface. The propagation of the surface may be tracked by the field variable  $\tilde{G}$  and the flame front is taken as the iso-level  $\tilde{G} = G^*$ . Where,  $G^*$  is often defined to be zero. The interesting fact is that the resolved  $\tilde{G}$  field does not have to follow the progress variable gradient. It can be smoothed out in space as broad as several mesh elements so that it may be resolved on the LES mesh. Simulation of  $\tilde{G}$  field requires the solution of a transport equation where the displacement speed is modelled using the turbulent flame speed [13]. The major difficulty is that the turbulent flame speed is yet not a well-defined quantity and no universal model formulation can be found. Several geometrical assumptions also have to be imposed to maintain the adequate simplicity of the model while artificial diffusivity has to be added to avoid numerical difficulties arising due to the formation of flame cusps [14, 15]. Therefore the successful integration of the level set formulation with the turbulent flow field also requires considerable research.

The thicken flame model [16], artificially enhances the flame front thickness so that it can be sufficiently resolved in the computational mesh. Thickening of the flame front could be achieved by multiplying the thermal diffusivity by a user defined factor  $F$ , as the flame thickness  $\delta_L$  is given by the ratio between the thermal diffusivity and the laminar flame speed. However, it is required to maintain the true laminar flame propagation speed so that a correction for the reaction rate is required. Simple laminar flame theories suggest that the laminar flame speed is proportional to the product of thermal diffusivity and the pre-exponential factor of the Arrhenius reaction rate equation. Hence, correct reaction rate is achieved by dividing the pre-exponential factor by the same factor  $F$ . The major advantage of this formulation is that it can be used to study various phenomena such as ignition and wall flame interaction, without the use of ad-hoc sub models as the reaction rate is modelled using the Arrhenius law [17]. Applications of this model for gas turbine combustion analysis [18, 19] and SI engines [20] have been reported. Extension of this study to analyse cyclic variations of combustion instabilities in SI engine combustion has also been reported in [21]. However, since the use of this method is combined with Arrhenius type reaction model, the flame region has to be accurately resolved for a reasonable solution. On the other hand, the thicken flame model requires the use of a combustion filter width, which is at least larger than 10 times the cell size (the classical LES filter width). For better

results this can be up to fifty times [17]. Hence, compared to the other methods, thicken flame approach is more demanding in terms of the mesh resolution requirement [22].

Another interesting approach to solve the flame thickness problem is to filter the progress variable (or species mass fraction) by a larger filter size than the classical LES filter width [23]. The present study is based on this technique and uses the flame surface density (FSD) model as further explained in the following sections. In this work, attempts have also been made to develop an LES based dynamic procedure for turbulent premixed combustion calculations in spark ignited gasoline engines. The work is based on the well-known KIVA-4 code. It is the latest of RANS based CFD flow solvers of KIVA series, capable of simulating three-dimensional, multispecies gaseous flows under steady and transient conditions. KIVA solves the governing equations in an Arbitrary Lagrangian Eulerian framework and has the ability to handle unstructured meshes with moving boundaries. In this study, the code was extensively modified to incorporate LES capability by implementing a sub-grid scale turbulence model, where a separate transport equation is solved for the sub-grid kinetic energy. An improved model for the spark ignition and flame kernel formation in the LES context was also developed. Fully developed phase of the combustion was simulated using a dynamic flame surface density approach. Full cycle simulations were carried out for a number of engine cycles and predictions were compared against experimentally measured data for the same engine.

## NUMERICAL PROCEDURE

Described in this section are the Favre filtered governing equations solved during the present study for a premixed reacting flow field. A comprehensive discussion on the derivation of these equations can be found in [24, 25]. Specific aspects of implementation into the KIVA-4 code is explained in [26]. The momentum equation applied in the  $x$  direction for example, can be written as:

$$\begin{aligned} \frac{\partial}{\partial t}(\bar{\rho}\tilde{u}) + \nabla \cdot (\bar{\rho}\tilde{u}\tilde{U}) + \nabla \cdot \tau_{sgs,x} \\ = -\frac{\partial \bar{p}}{\partial x} + \frac{\partial \bar{\tau}_{xx}}{\partial x} + \frac{\partial \bar{\tau}_{yx}}{\partial y} + \frac{\partial \bar{\tau}_{zx}}{\partial z} \end{aligned} \quad (1)$$

where,  $U$  is the velocity vector and  $u$  is its component in  $x$  direction,  $\rho$  is the fluid density and  $p$  is the pressure. The SGS tensor is denoted by  $\tau_{sgs}$  and  $\tau_{sgs,x}$  corresponds to its components in  $x$  direction.  $\tau_{yx}$  indicates the stress component acting in  $y$  plane in  $x$  direction. The resolved stress tensor  $\tau$  can be obtained by filtering the Newtonian stress tensor as:

$$\tau = \mu \left[ (\nabla \otimes \tilde{U}) + (\nabla \otimes \tilde{U})^T \right] - \frac{2}{3} \mu (\nabla \cdot \tilde{U}) \mathbb{I} \quad (2)$$

where,  $\mathbb{I}$  is the unit tensor and  $\mathbb{T}$  is the transpose.  $\mu$  represents the dynamic viscosity and  $\otimes$  denotes the tensor product. The closure of the momentum equation requires an expression for the SGS stress tensor. In this study, an approach based on the SGS kinetic energy:  $k_{sgs}$ [24], is taken.

The assembled SGS stress tensor can be given by:

$$\tau_{sgs} = -\mu_{sgs} \left[ (\nabla \otimes \tilde{U}) + (\nabla \otimes \tilde{U})^T \right] + \frac{2}{3} [(\nabla \cdot \tilde{U}) + \bar{\rho} k_{sgs}] \mathbb{I} \quad (3)$$

The SGS viscosity:  $\mu_{sgs}$ , is evaluated by the following expression.

$$\mu_{sgs} = C_v \bar{\rho} k_{sgs}^{1/2} \bar{\Delta} \quad (4)$$

$C_v$  is a model constant usually taken to be 0.067 for engine configurations [24,27]. SGS kinetic energy is obtained by solving the following transport equation.

$$\begin{aligned} \frac{\partial}{\partial t} (\bar{\rho} k_{sgs}) + \nabla \cdot (\bar{\rho} k_{sgs} \tilde{U}) \\ = -(\nabla \otimes \tilde{U}) : \bar{\tau}_{sgs} - D_{sgs} \\ + \nabla \cdot \left( \frac{\mu_{sgs}}{Sc_k} \nabla k_{sgs} \right) \end{aligned} \quad (5)$$

Balance equations for the species and global mass conservation can be specified as:

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{U}) = 0 \quad (6)$$

$$\begin{aligned} \frac{\partial (\bar{\rho} \tilde{Y}_m)}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{Y}_m \tilde{U}) - \nabla \cdot \left( \frac{\mu}{Sc} \nabla \tilde{Y}_m \right) + \nabla \cdot \Phi_{sgs} \\ = \bar{\rho}_{m,c} \end{aligned} \quad (7)$$

$$\Phi_{sgs} = - \left( \frac{\mu_{sgs}}{Sc_{sgs}} \nabla \tilde{Y}_m \right) \quad (8)$$

where,  $Y_m$  is the mass fraction of species  $m$ . The unresolved convective fluxes are denoted by  $\Phi_{sgs}$  and closed using the classical gradient assumption.  $\bar{\rho}_{m,c}$  denotes the source term due to combustion. Similarly, the transport of specific internal energy  $I$  can be written as:

$$\begin{aligned} \frac{\partial}{\partial t} (\bar{\rho} I) + \nabla \cdot \bar{\rho} I \tilde{U} + \bar{p} (\nabla \cdot \tilde{U}) + \nabla \cdot \bar{q} - (\nabla \otimes \tilde{U})^T : \bar{\tau} \\ + \nabla \cdot h_{sgs} - D_{sgs} = \bar{Q}_{l,c} \end{aligned} \quad (9)$$

$$h_{sgs} = - \frac{\mu_{sgs} c_p}{Pr_{sgs}} \nabla \cdot \tilde{T} \quad (10)$$

$$D_{sgs} = C_\varepsilon \bar{\rho} k_{sgs}^{3/2} / \bar{\Delta} \quad (11)$$

where,  $h$  is the enthalpy and  $T$  is the temperature.  $\bar{Q}_{l,c}$  is the combustion source term and  $c_p$  is the specific heat capacity at constant pressure.  $D_{sgs}$  represents the rate of dissipation of SGS kinetic energy.

The heat flux vector  $q$  is given by:

$$\bar{q} = -\mathcal{K}(\nabla \tilde{T}) - \sum_m \frac{\mu}{Sc} \tilde{h}_m (\nabla \tilde{Y}_m) \quad (12)$$

$\mathcal{K}$  is the thermal conductivity of the fluid mixture and the summation is over all the species.

The LES filter width is taken as:

$$\bar{\Delta} = (\Delta x \Delta y \Delta z)^{1/3} \quad (13)$$

where,  $\Delta x$ ,  $\Delta y$  and  $\Delta z$  are length, width and height of the computational cell, thus the cut off scale is often taken equivalent to the cubic root of the cell volume. Rest of the modelling constants were assigned the following values following [24].  $C_\varepsilon = 0.916$   $Sc_k = 1.0$   $Pr_{sgs} = 0.9$   $Sc_{sgs} = 0.9$ . The implementation of this model in the KIVA-4 code has been successfully validated with respect to experimental and DNS data as reported in [26].

## Modelling the Reaction Rate Using a FSD Approach

It is also possible to extend the FSD concept; i.e  $\Sigma$  : the available flame surface area for unit volume, developed in RANS to perform combustion calculations in LES, in conjunction with the filtered balance equation of progress variable or species mass fractions [10]. However, as already pointed out, the stiffness associated with the spatial distribution in progress variable has to be eliminated in order this method to be successful.

### Combustion filter width

It has been demonstrated that if the flame front is filtered with a larger filter size  $\bar{\Delta}_c$  than the classical LES filter width  $\bar{\Delta}$ , a similar effect can be seen as the thickened flame model [23]. For example, if the combustion filter width  $\bar{\Delta}_c$  is taken to be 4 times the grid filter width  $\bar{\Delta}$ , the progress variable gradient is dispersed over  $2\bar{\Delta}_c/\bar{\Delta}$  grid points ( $2\bar{\Delta}_c/\bar{\Delta} = 8$  in this case). In practice, the flame front is thickened by a factor in the order of  $\bar{\Delta}_c/\delta_L$  [22] making it possible to resolve with a sufficiently large filter width.

The resolution parameter  $\eta_{res}$  is defined by relating combustion and grid filter widths as:

$$\bar{\Delta}_c = \eta_{res} \bar{\Delta} \quad (14)$$

It has also been highlighted in [23] that there should be at least eight grid points for the accurate solution of the flame front. Therefore in practice  $\eta_{res}$  is chosen such that  $5 < \eta_{res} < 10$  [9].

It should be noted here that the filter width  $\bar{\Delta}_c$  is applied only to the flame region and for the rest of the domain the classical filter width  $\bar{\Delta}$  must be used. In addition,  $\bar{\Delta}_c$  is used only with the species (or progress variable) and enthalpy transport equations. In the momentum equations,  $\bar{\Delta}$  is used all over the domain including the flame front region. In a practical CFD simulation it is difficult to exactly identify a flame region, therefore the combustion filter width may be used only in the region where filtered progress variable  $10^{-3} \leq \tilde{c} \leq 1 - 10^{-3}$  as recommended in [9].

Use of the filter width in governing equations is associated with the calculation of the SGS viscosity. Hence, the SGS viscosity in the flame region  $\mu_{sgs-c}$ , has to be calculated as follows.

$$\mu_{sgs-c} = C_v \bar{\rho} k_{sgs-c}^{1/2} \bar{\Delta}_c \quad (15)$$

where,  $k_{sgs-c}$  is taken as:

$$k_{sgs-c} = k_{sgs} \left( \frac{\bar{\Delta}_c}{\bar{\Delta}} \right)^{2/3} \quad (16)$$

assuming Kolmogorov energy cascade in the inertial sub range. Consequently, the balance equation for mass fraction, enthalpy or progress variable have to be modified to incorporate combustion filter scale viscosity as given in the form below for a general scalar  $\phi$ .

$$\frac{\partial \bar{\rho} \tilde{\phi}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\phi} \tilde{U}) - \nabla \cdot \left[ \left( \frac{\mu}{Sc} + \frac{\mu_{sgs-c}}{Sc_{sgs}} \right) \nabla \tilde{\phi} \right] = S_\phi(\bar{\Delta}_c) \quad (17)$$

Also, it is worth mentioning that the combustion source term in the above equation is a function of the combustion filter width  $\bar{\Delta}$ .

### Transport of the progress variable

The modified equation suggested in [28] for the Favre filtered progress variable:  $\tilde{c}$  is adopted in the present study to solve for the species mass fraction  $\tilde{Y}_m$ .

$$\begin{aligned} & \frac{\partial (\bar{\rho} \tilde{Y}_m)}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{Y}_m \tilde{U}) \\ & + \nabla \cdot \left[ \left( \rho_u \frac{S_L \bar{\Delta}_c}{16\sqrt{6/\pi}} + \frac{\mu_{sgs-c}}{Sc_{sgs}} \right) \nabla \tilde{Y}_m \right] \\ & = \langle \rho_u \tilde{Y}_m S_D \rangle_S \bar{\Sigma} \end{aligned} \quad (18)$$

where,  $\bar{\Sigma} = |\nabla \tilde{c}|$  denotes a generalized filtered flame surface density and, is a measure of total flame surface area contained within the filtered volume. The density weighted surface averaged displacement speed  $\langle \rho S_D \rangle_S$  is generally approximated in terms of the unburned gas density  $\rho_u$ , and laminar flame speed  $S_L$ .

$$\langle \rho S_D \rangle_S = \rho_u S_L \quad (19)$$

$\bar{\Sigma}$  can be evaluated by solving a balance equation for the transport of flame surface density, making necessary allowance for the unresolved contribution [9,29]. However, these models often involve several model constants which need to be specified on case by case basis. Alternatively, a simpler but an attractive approach is to use an algebraic model formulation which may only have one or two calibration constants. The algebraic model developed here, virtually involve no adjustable constant, as they are dynamically estimated using the resolved scale information. In fact, the potential of dynamic algebraic formulations in predicting reacting SI engine flows have never been tested. Thus, with the aim of gaining confidence in premixed turbulent combustion in SI engines the, the present work adopts an algebraic FSD formulation.

### A Flame Kernel Growth Model

Combustion characteristics during the early stage of kernel formation, is fundamentally different from its fully developed phase [8, 30]. Flame has not achieved equilibrium and flame propagation is mainly affected by volumetric expansion. Instead, as the flame kernel remains smaller than the computational mesh during the early stage of propagation, the flame front cannot be resolved in the computational mesh [31]. Thus, combustion models, usually developed with equilibrium assumptions for fully developed flames are not valid for this stage and specific modifications are needed. Only a very limited amount of work has been carried out in LES context, on ignition and flame kernel formation in SI engines. In [31] and [32], FSD transport equation based ignition models have been developed considering aforementioned aspects. Recently, an experimentally based comprehensive formulation combined with the G-equation approach has also been proposed in [33] and [34] for RANS simulations. This would, probably be easily extended in to LES, in a LES G-equation formulation. However, in the present work, a simple model, but effectively capable of producing global results of ignition and early stage of flame propagation is proposed.

### Initiation of the ignition kernel

The most accurate method to initiate the ignition is to impose a plasma channel, based on the characteristics of the electrical system and in-cylinder mixture properties. Solving for the complex plasma physics is usually a formidable task. Hence, in the present approach the flame kernel is initiated by