

A Transport Equation Residual Model Incorporating Refined G-Equation and Detailed Chemical Kinetics Combustion Models

Shiyou Yang and Rolf D. Reitz
University of Wisconsin-Madison

Claudia O. Iyer and Jianwen Yi
Ford Research & Advanced Engineering

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ABSTRACT

A transport equation residual model incorporating refined G-equation and detailed chemical kinetics combustion models has been developed and implemented in the ERC KIVA-3V release2 code for Gasoline Direct Injection (GDI) engine simulations for better predictions of flame propagation. In the transport equation residual model a fictitious species concept is introduced to account for the residual gases in the cylinder, which have a great effect on the laminar flame speed. The residual gases include CO_2 , H_2O and N_2 remaining from the previous engine cycle or introduced using EGR. This pseudo species is described by a transport equation. The transport equation residual model differentiates between CO_2 and H_2O from the previous engine cycle or EGR and that which is from the combustion products of the current engine cycle. The refined G-equation and detailed chemical kinetics include revision of a PRF chemistry mechanism, and introduction of a Damkohler criterion which determines whether the G-equation model or chemical kinetics should be used for assessing the combustion processes in flame-containing cells. Validation of the revised PRF mechanism shows that the calculated ignition delay matches shock tube data very well. The Damkohler criterion is based on a comparison between a laminar flame propagation time scale and the chemical kinetics time scale, and the results from implementation of the Damkohler model range between the G-equation model and pure chemistry, depending on the conditions. The integrated model was used to simulate the combustion process in a Gasoline Turbocharged Direct Injection (GTDI) engine, and the same set of combustion model parameters for both high load and low load were used. For both high load and low load operating conditions, good agreement with experimental in-cylinder pressure, heat release rates and Mass Fraction Burned (MFB) data was obtained.

INTRODUCTION

Multidimensional Computational Fluid Dynamics (CFD) modeling is a powerful tool to investigate and analyze phenomena occurring in the internal combustion engine. In recent times, CFD has been widely used for the design of internal combustion engines for the purpose of obtaining low emissions and increasing fuel efficiency. An important CFD code which has been used extensively for modeling internal combustion engines is the KIVA code [1-5]. Understanding the in-cylinder ignition and combustion processes is one of the key factors for successful modeling. The in-cylinder turbulent ignition and combustion process in Spark Ignition (SI) engines is a complicated aero-thermo-chemical process, especially due to the turbulence and chemistry interactions that occur on tremendously different time-scale and length-scale levels [6,7]. To better model the ignition process, a Discrete Particle Ignition Kernel model (DPIK), in which the flame kernel position is marked by particles, was proposed by Fan and Reitz [8]. The level set method (G-equation) is a powerful tool to model both premixed and partially premixed combustion occurring in SI engines. With its application to combustion, Williams [9] first suggested use of a transport equation for a non-reactive scalar, G , for laminar flame propagation. Peters [7,10] subsequently extended this approach to the turbulent flame regime. The turbulent G-equation concept has been successfully applied to SI engine combustion simulations by Dekena et al. [11], Tan [12], and Ewald et al. [13].

To better understand the fundamental engine combustion process and to further improve the versatility of multidimensional models, attention is being given to models incorporating comprehensive elementary chemical kinetics mechanisms. A large amount of work has been done on developing detailed chemical kinetics mechanisms for fuel oxidation and pollutant formation [14]. Further, research on mechanism reduction and parallel computing techniques has made it computationally affordable to incorporate these reduced detailed chemical kinetics mechanisms into

multidimensional engine simulations. Liang [15,16,17] successfully incorporated detailed chemical kinetics into the G-equation-based turbulent combustion model, which was implemented into the KIVA-3V release2 code by Tan et al. [18,19]. Specifically, for SI engine combustion, detailed fuel oxidation mechanisms coupled with a reduced NO_x mechanism are applied behind the mean flame front for modeling post flame combustion and NO_x formation. The chemical kinetics mechanisms are also applied in front of the flame front for predicting compression auto-ignition of the end-gas (knock). Also in Liang's work, in the course of coupling detailed chemistry with the G-equation combustion model for the primary heat release calculation within the flame front, the laminar and turbulent flame speed correlations were improved for a better description of the turbulent flame propagation process.

In the G-equation-based turbulent combustion model the laminar flame speed is very important for determining the propagation of the flame front ($G=0$) surface. Also, the local and instantaneous residual value has a great effect on the evaluation of the laminar flame speed. For the calculation of the residual value, Yang et al. [20] used several different empirical methods.

In this paper, we present a transport equation residual model incorporating refined G-equation and detailed chemical kinetics combustion models for Gasoline Direct Injection (GDI) engine combustion simulations. In the transport equation residual model a fictitious species is introduced to account for the residual gases in the cylinder. The evolution of the pseudo species is described by a transport equation. The refined G-equation and detailed chemical kinetics combustion models include a revision of the PRF chemistry mechanism, use of a Damkohler criterion, in which a comparison between a laminar flame propagation time scale and a chemical kinetics time scale determines whether the G-equation model or chemical kinetics will be used to fundamentally determine the combustion processes in flame-containing cells. Finally, we present simulation results of the integrated model applied to model the combustion process in a Gasoline Turbocharged Direct Injection (GTDI) engine.

G-EQUATION DESCRIPTION OF MODELING PREMIXED TURBULENT FLAME PROPAGATION

A G-equation combustion model for describing turbulent flame propagation has been developed and implemented into the KIVA-3V release2 code by Tan and Reitz [18,19]. Subsequently, consideration of detailed chemical kinetics was incorporated into the KIVA-3V release2 G-equation code to model the post-flame chemistry and end-gas auto-ignition chemistry by Liang and Reitz [15,16,17]. The G-equation combustion model is mainly based on the turbulent premixed combustion flamelet theory by Peters [7], where a set of Favre-averaged level-set equations was derived, including equations for the Favre mean, $\tilde{G}$, and its variance, $\tilde{G}''^2$, and a model equation

for the turbulent/laminar flame surface area ratio σ_T , which, in turn, results in an explicit expression for the turbulent flame speed S_T^0 . These equations, together with the Reynolds averaged Navier-Stokes equations and the turbulence modeling equations, form a complete set to describe premixed turbulent flame front propagation. The equation set suitable for implementation in CFD codes is [7,15,19]:

$$\frac{\partial \tilde{G}}{\partial t} + (\tilde{u} - \tilde{u}_{vertex}) \cdot \nabla \tilde{G} = \frac{\bar{\rho}_u}{\bar{\rho}} S_T^0 |\nabla \tilde{G}| - D_T \tilde{k} |\nabla \tilde{G}|, \quad (1)$$

$$\frac{\partial \tilde{G}''^2}{\partial t} + \tilde{u} \cdot \nabla \tilde{G}''^2 = \nabla_{||} \cdot \left(\frac{\bar{\rho}_u}{\bar{\rho}} D_T \nabla_{||} \tilde{G}''^2 \right) + 2 D_T (\nabla \tilde{G})^2 - c_s \frac{\tilde{\varepsilon}}{\tilde{k}} \tilde{G}''^2, \quad (2)$$

$$\frac{S_T^0}{S_L^0} = 1 + I_p \left\{ -\frac{a_4 b_3^2 l_l}{2 b_1 l_f} + \left[\left(\frac{a_4 b_3^2 l_l}{2 b_1 l_f} \right)^2 + a_4 b_3^2 \frac{u' l_l}{S_L^0 l_f} \right]^{1/2} \right\}, \quad (3)$$

where $\tilde{G}$ is the Favre-average of G ; $\tilde{G}''^2$ is the variance of $\tilde{G}$; $\tilde{u}$ is the Favre-average fluid velocity; $\tilde{u}_{vertex}$ is the mesh vertex velocity which accounts for mesh movement; $\nabla \tilde{G}$ is the gradient of $\tilde{G}$; $\nabla \tilde{G}''^2$ is the gradient of $\tilde{G}''^2$; $\bar{\rho}_u$ is the Reynolds-average of the unburned mixture density; $\bar{\rho}$ is the Reynolds-average of the cell gas density; S_T^0 is the turbulent flame speed; D_T is the turbulent diffusivity; $\nabla_{||}$ denotes the tangential gradient operator; c_s is a modeling constant (cf. Ref. [7]); $\tilde{k}$ and $\tilde{\varepsilon}$ are the Favre mean turbulent kinetic energy and its dissipation rate from the RNG $k-\varepsilon$ model [21]; u' is the turbulence intensity; S_T^0 is the turbulence flame speed; S_L^0 is the laminar flame speed; l_l and l_f are the turbulence integral length scale and the laminar flame thickness, respectively; and a_4 , b_3 , b_1 are constants from turbulent flame speed model [7]. The term I_p in Eq. (3), called a progress variable in Ref. [15], takes the form

$$I_p = \left[1 - \exp(-c_{m2} \frac{t - t_0}{\tau}) \right]^{1/2}, \quad (4)$$

where c_{m2} is a model constant; t_0 is the spark timing; $\tau = \tilde{k} / \tilde{\varepsilon}$ is the turbulence time scale. Physically, the progress variable I_p models the increasingly disturbing effect of the surrounding eddies on the flame front surface as the spark-ignition kernel flame grows from the laminar stage into the fully developed turbulent stage.

THE EFFECT OF RESIDUAL ON FLAME SPEED

The laminar flame speed correlation used is [Ref. 15]:

$$S_L^0 = S_{L,ref}^0 \left(\frac{T_u}{T_{u,ref}} \right)^\alpha \left(\frac{p}{p_{ref}} \right)^\beta F_{dil} \quad (5)$$

where $S_{L,ref}^0$ is the laminar flame speed at a reference state, T_u is the unburned mixture temperature, $T_{u,ref}$ is the unburned mixture temperature at the reference state, p is the pressure, p_{ref} is the reference pressure, and α and β are correlated as functions of equivalence ratio. F_{dil} is a factor that accounts for the presence of diluents, which can be expressed as:

$$F_{dil} = 1 - f_{dil} Y_{dil} \quad (6)$$

where f_{dil} is an experimentally determined constant, and Y_{dil} is the "residual mass fraction", including CO_2 , H_2O , residual N_2 , and other residual components. From the above correlations, it is seen that the turbulent flame speed S_T^0 decreases as the "residual mass fraction" Y_{dil} increases and the evaluation of turbulent flame speed is sensitive to the "residual mass fraction".

The effect of residual value on the flame speed can be seen in Figure 1 [22] and Figure 2 [23].

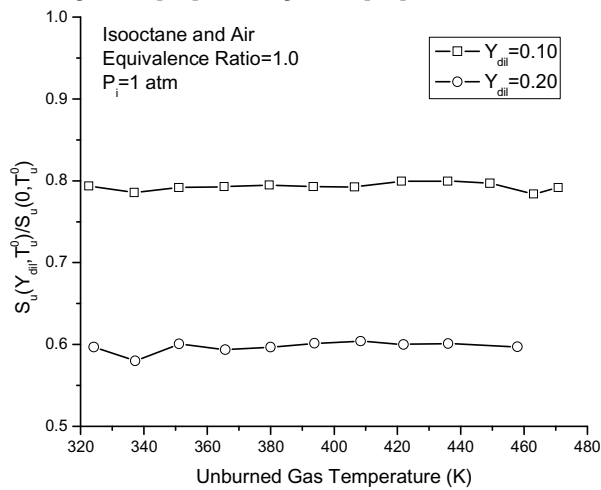


Figure 1 Effect of diluting stoichiometric isooctane-air mixtures with simulated combustion products [22]

In Metghalchi and Keck's work, as shown in Figure 1, the effect of diluting stoichiometric isooctane-air mixtures with simulated combustion products was measured for an initial temperature $T_1=298\text{K}$ and $P_1=1\text{ atm}$. A mixture of 15% carbon dioxide and 85% nitrogen by volume was used to simulate combustion products. This mixture has a molecular weight of 30.4 and a heat capacity which approximately matches that of the combustion products. In Figure 1, the ratio of the burning velocities with and without dilution are plotted as a function of unburned gas temperature for diluent mass fractions $Y_{dil}=0.1$ and $Y_{dil}=0.2$. It can be seen that the decrease in burning velocity ratio is independent of temperature and can be represented by the expression

$$S_u(Y_{dil}, T_u^0) / S_u(0, T_u^0) = 1 - 2.1 Y_{dil} \quad (7)$$

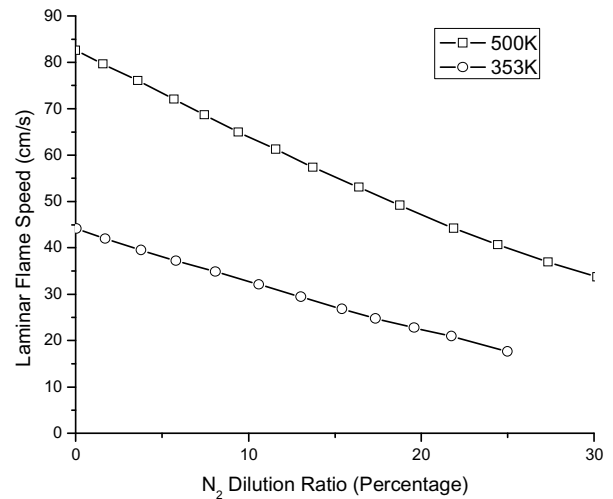
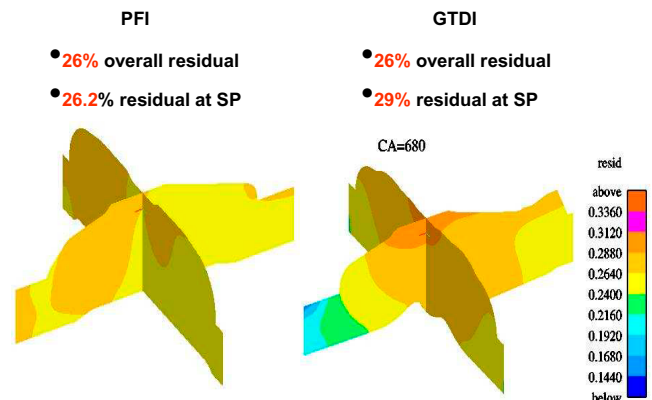


Figure 2 Laminar flame speed of 87 octane gasoline at atmospheric pressure with N_2 dilution for equivalence ratio of 0.84 at 353 K and 500 K [23]

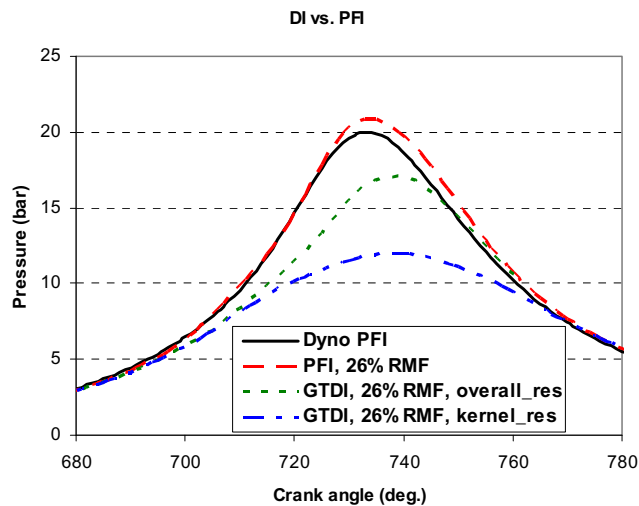
In Zhao et al.'s work, as shown in Figure 2, the dilution effect on the laminar flame speed was studied for 87 octane gasoline at 353 K and 500 K for equivalence ratio of 0.84 with N_2 as diluent. The laminar flame speeds in Figure 2 exhibit nearly linear dependencies on the dilution ratio.

For the engine simulation, the residual value of the cell at the location of the spark plug at the time of spark ignition was used in every cell in the combustion model of Liang [15,16,17]. However, the local and instantaneous residual value should be used for more accurate results.

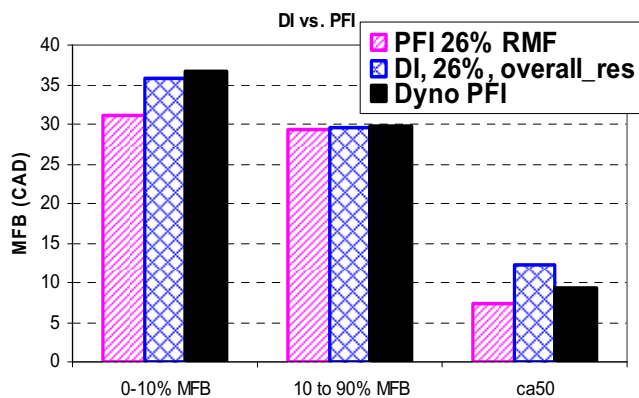
The effect of residual value on burning velocity for a real engine simulation is shown in Figure 3, from Yang et al. [20]. These computations were conducted by considering the full intake stroke (starting at intake valve opening) with mixing of the exhaust residual with the fresh gas.



(a) Residual value distribution



(b) Pressure comparison



(c) Burning rate comparison

Figure 3 Sensitivity of burning rate to residual gas distribution

Figure 3(a) shows the residual gas mass fraction distribution in the combustion chamber in two perpendicular planes at 40° before TDC. The left Figure 3(a) is for a Port Fuel Injection (PFI) engine at low load, whose mixture is nearly homogeneous. The overall residual value is 26%, which is nearly the same as the residual value of the cell at the location of the spark plug at the time of spark ignition (which is 26.2%). The right Figure 3(a) shows the residual gas distribution of a Gasoline Turbocharged Direct Injection (GTDI) engine at low load, whose mixture is stratified. The overall residual value is 26%, while the residual of the cell at the location of the spark plug at the time of spark ignition is 29%.

Figure 3(b) shows a predicted cylinder pressure comparison made using different residual values for both the PFI and GTDI cases. It should be noted that in the comparison all simulation conditions are kept the same except that different residual values are used. For the PFI case, when the residual value of the cell at the location of the spark plug at spark ignition is used (PFI, 26% RMF), the pressure curve matches the

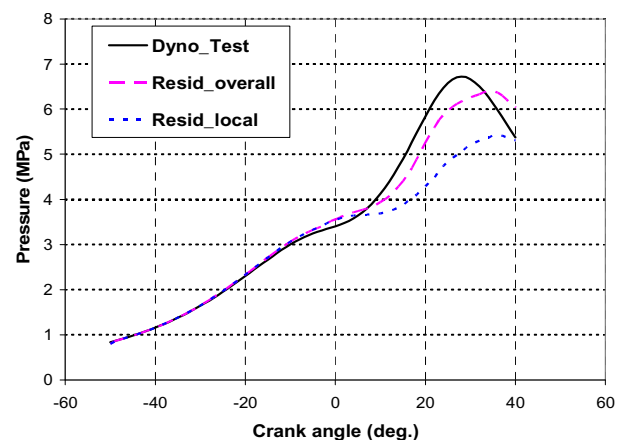
experimental data (Dyno PFI) since the residual value is close to the overall residual value. For the GTDI case, when the residual of the cell at the location of spark plug at spark ignition is used (GTDI, 26% RMF, kernel_res), the predicted pressure curve is much too low since the used residual value is greater than the overall residual value.

When the overall residual value is used for the GTDI case, the predicted pressure (GTDI, 26% RMF, overall_res) is increased and approaches the experimental data (which is close to “Dyno PFI”). Figure 3(c) shows burning rate comparisons for the different residuals for PFI and GTDI cases. From Figure 3(c) it is seen that for the PFI the 0~10% MFB from using the residual of the cell at the spark plug (PFI 26% RMF) is lower than the experimental data. All cases have nearly the same 10~90% MFB. For the GTDI case the ca50 using the overall residual value (DI, 26%, overall_res) is higher than the experimental data. From Figure 3 it can be concluded that although the use of the overall residual is better than the use of the residual value of the cell at the spark plug, the simulated results of the stratified GTDI case still do not match the experimental data, and thus it is reasonable to explain the use of the local and instantaneous residual value.

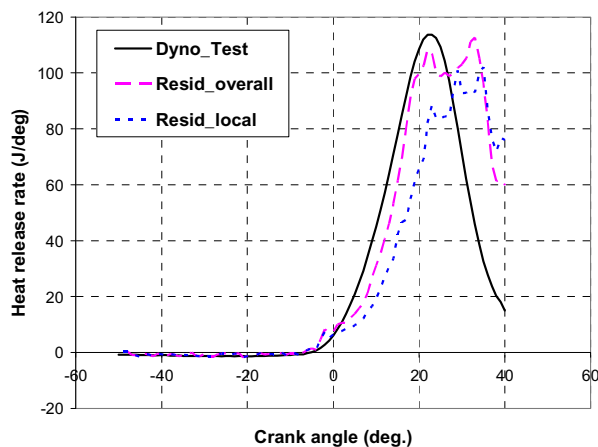
The local and instantaneous residual value is determined from

$$Y_{dil} = y_{co_2} (1 + 0.7273 * 3.29 * \alpha / 14.7) + y_{h_2o} (1 + 0.8889 * 3.29 * \alpha / 14.7) \quad (8)$$

where y_{co_2} is the mass fraction of CO_2 ; $0.7273 * 3.29$ is the corresponding stoichiometric N_2 amount; α is the local air fuel ratio; 14.7 is the stoichiometric air fuel ratio for gasoline; The terms including H_2O are similar to those of CO_2 .



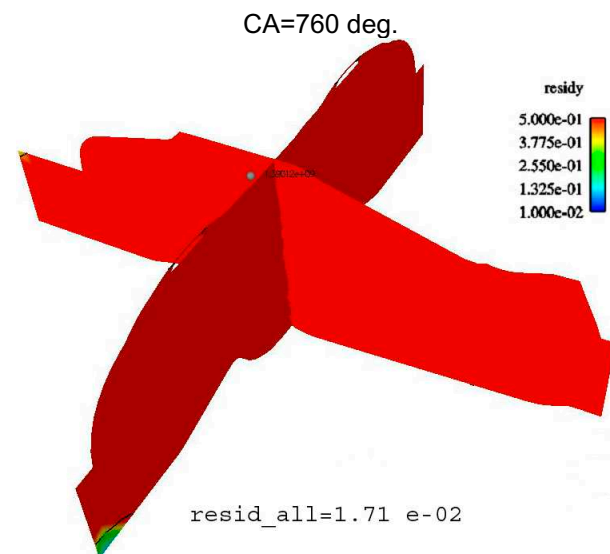
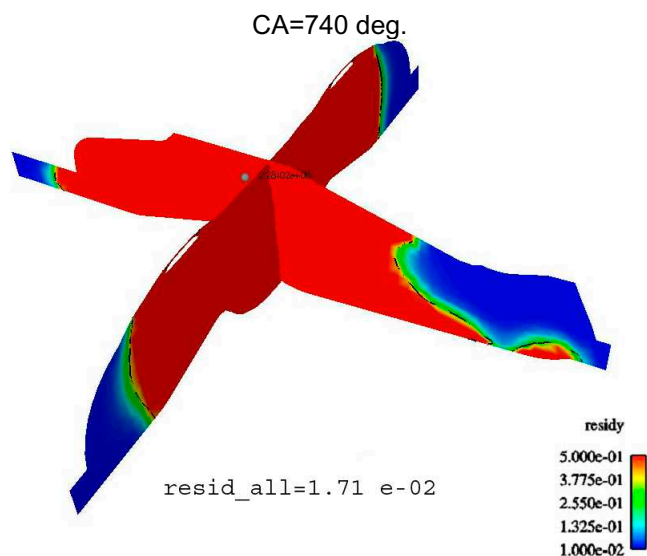
(a) Pressure



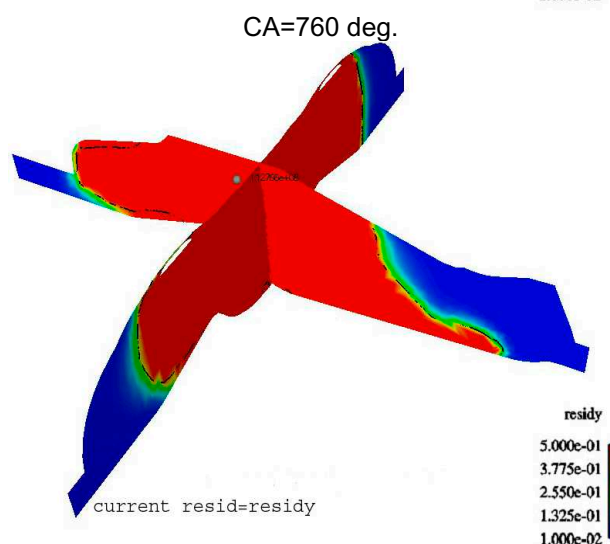
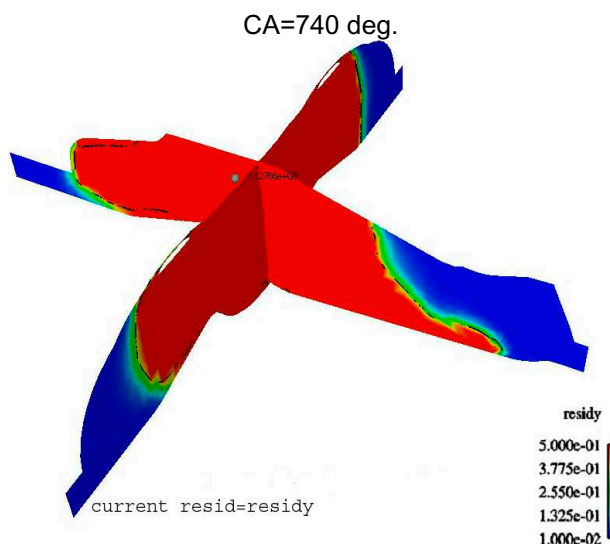
(b) Heat release rate

Figure 4 Predicted cylinder pressure and heat release rate considering overall and local residual

Figures 4(a,b) show the results when the local and instantaneous residual is considered for the GTDI engine at high load (boosted, 2000 rev/min). Both the pressure and heat release rate predicted using the local and instantaneous residual value are even worse than those using the overall residual value. Figures 5(a,b) show comparisons of the residual gas mass fraction distribution and the flame front propagation using the overall residual value method and the local and instantaneous residual value. "Residy" means the local residual, and "resid_all" means overall residual. In Figure 5, the black curve denotes the flame front "G=0" surface. From Figure 5 it is seen that at the same crank angle, e.g., 760° CA, the "flame front" surface (black curve) of the overall residual value method reaches the combustion chamber liner wall, while using the local and instantaneous residual the flame propagation is much reduced.



(a) Overall residual method



(b) Local and instantaneous residual method

Figure 5 Residual gas mass fraction distribution and flame front propagation

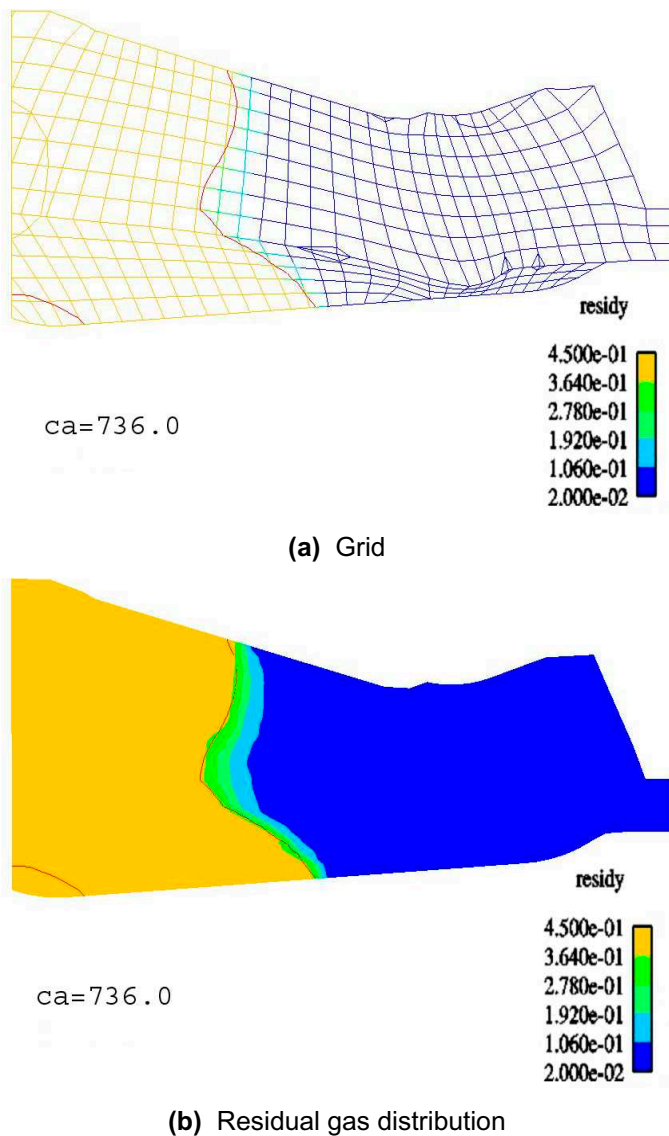


Figure 6 Grid and corresponding local and instantaneous residual gas distributions

Figure 6 shows the mesh in a diametral plane through the cylinder center line and the corresponding local and instantaneous residual mass fraction distribution. In both (a) and (b) of Figure 6, the red curve denotes the flame front “G=0” surface. When the local and instantaneous

residual mass fraction correlation is used, the value of residual in the cell in front of the flame front is used to compute the flame speed. From Figure 6 it is seen that the value in the cell just in front of the “G=0” surface is around 10%–30%, while the overall residual value for this engine operating condition is approximately 2.0%. This high local and instantaneous residual value in front of the flame front is due to either numerical or physical diffusion of the high concentrations of burned gas products behind the flame front region. Although typical flamelet models assume that there is no leakage of products across the flame surface (treated as infinitely thin) to the end gas, in KIVA calculation a flame containing cell is just computed as a whole, and it is hard to separately compute unburned side and burned side in the flame containing cell with KIVA-3V version. This is the reason why the flame speed slows down when the local and instantaneous residual is used.

TRANSPORT EQUATION RESIDUAL MODEL

Yang et al. [20] explored different methods to calculate the “residual mass fraction”, including using the residual value of the cell at the location of the spark plug at the time of spark ignition and the overall residual value of the cylinder, which have been mentioned earlier. Then they used a new method to account for the local residual mass fraction. In this new method (called “Resid_save”) the local residual mass fraction distribution in the combustion chamber before spark ignition is stored into an array. Then during combustion, the stored local residual mass fraction for each cell is used to calculate the flame speed. The results showed that the “Resid_save” method was better than others. However this method only considers the “local” characteristics of the residual, and it does not consider the transport either by diffusion or by convection and source terms of residual. That means it does not consider the “instantaneous” characteristics of residual. To accurately calculate the residual value distribution and to distinguish between burned gas combustion products that originate from the EGR gases and those from the current combustion event, considering the following cases: a transport equation residual model is used, which will be described in detail in the following sections.