

# Improvements to Combustion Models for Modeling Spark-Ignition Engines Using the G-equation and Detailed Chemical Kinetics

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

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

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## ABSTRACT

Improvements to combustion models for modeling spark ignition engines using the G-equation flame propagation model and detailed chemical kinetics have been performed. The improvements include revision of a PRF chemistry mechanism, precise calculation of “primary heat release” based on the sub-grid scale unburned/burnt volumes of flame-containing cells, modeling flame front quenching in highly stratified mixtures, introduction of a Damkohler model for assessing the combustion regime of flame-containing cells, and a better method of modeling the effects of the local residual value on the burning velocity. The validation of the revised PRF mechanism shows that the calculated ignition delay matches shock tube data very well. The improvements to the “primary heat release” model based on the cell unburned/burnt volumes more precisely consider the chemical kinetics heat release in unburned regions, and thus are thought to be physically reasonable. The simulation results show that the flame front quenching model effectively captures the flame quench phenomenon in highly stratified mixtures which are typical in Gasoline Direct Injection (GDI) engines. The results from implementation of the Damkohler model range between the G-equation model and pure CHEMKIN, depending on the conditions. Finally, an improved method is proposed to calculate the effects of local residual values on flame speed. After using these combined improvements to the combustion model, calibrations from high load to low load were applied to a Gasoline Turbocharged Direct Injection (GTDI) engine, and the same set of combustion model parameters for both high load and low load were used. The calibration results show that the simulated pressure, heat release rate, and Mass Fraction Burned (MFB) match the experimental data very well.

## 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 Dekema 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 mechanisms 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 release 2 code by Tan et al. [18,19]. Specifically, for SI engine combustion, detailed fuel oxidation mechanisms coupled with a reduced NO<sub>x</sub> mechanism are applied behind the mean flame front for modeling post flame combustion and NO<sub>x</sub> 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 this paper, we focus on further improvements to the G-equation combustion models with detailed chemical kinetics used for the modeling of spark ignition engines. The improvements to the combustion model include a revision of the PRF chemistry mechanism, precise calculation of "primary heat release" based on the sub-grid scale unburned/burnt volumes of flame-containing cells, modeling flame front quenching in highly stratified mixtures, use of a Damkohler criterion for flame-containing cells, and formulating a better method to model the effects of local residual gas levels on the burning velocity.

## DESCRIPTION OF IMPROVEMENTS TO COMBUSTION MODELS

### MODELING PREMIXED TURBULENT FLAME PROPAGATION

A G-equation combustion model for describing turbulent flame propagation has been developed and implemented into the KIVA-3V release 2 code by Tan and Reitz [18,19]. Subsequently, consideration of detailed chemical kinetics was incorporated into the KIVA-3V release 2 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  $\sigma_T$ , 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]:

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

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

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

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;  $\bar{u}_{vertex}$  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;  $\nabla_{\parallel}$  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 [20];  $u'$  is the turbulence intensity;  $S_T^0$  is the turbulence flame speed;  $S_L^0$  is the laminar flame speed;  $l_I$  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.

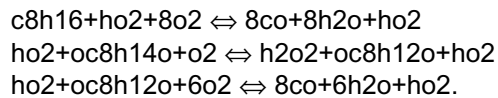
### IMPROVEMENT TO MODELING OF CHEMICAL KINETICS

As mentioned earlier, detailed chemistry is used to simulate the low-temperature auto-ignition process of the end-gas. Each computational cell ahead of the flame front is modeled as a WSR (Well-Stirred-Reactor) for calculating the chemistry source terms of the species and energy transport equations. The WSR approximation is based on the consideration that sharp gradients of temperature and species densities are not likely to exist within the end-gas zone during the low-temperature heat release stage. In addition, the WSR approximation has been proven to be an effective way of modeling HCCI combustion in several previous studies [21,22]. In the present model, the CHEMKIN

code [23] was used for solving the detailed chemical kinetics mechanisms.

In Liang's study [15,16,17], a 22-species, 42-reactions *iso*-octane ( $iC_8H_{18}$ ) mechanism, which was extracted from a 32-species, 55-reactions primary reference fuel (PRF) mechanism by Tanaka et al. [24], was adopted to model the auto-ignition process of the gasoline/air/residual-gas mixture ahead of the flame front in gasoline SI engines. This PRF mechanism was originally validated in a rapid compression machine (RCM) for fuel-lean mixtures over a wide range of initial temperature and pressure conditions, where the maximum equivalence ratio studied was 0.5 [24]. In Liang's work [15,16,17], the mechanism was further reduced and further validated for both lean and rich mixtures by comparing calculated ignition delay times with experimental data obtained from the shock-tube measurements by Fieweger et al. [25].

However the match of ignition delay between the experimental data and simulation results was not good, especially for rich mixtures. In the present study it was found that three reactions essentially control the ignition delay. The three reactions are:



The rates of the three reactions were revised and the new mechanism was validated with the shock tube data. The specific reaction rates of the new mechanism are presented in the model validation section of this paper. Also the ignition delay results from the old and new mechanisms are compared.

#### IMPROVEMENT TO "PRIMARY HEAT RELEASE" MODEL BASED ON SUB-GRID SCALE UNBURNED/BURNED VOLUMES OF FLAME-CONTAINING CELLS

##### (1) Model description

For turbulent premixed or partially premixed flames in SI engines, the heat release due to turbulent flame front propagation (called "primary heat release" in the present study) constitutes a major portion of the total in-cylinder heat release. In previous implementations of the G-equation model, it was assumed that with the propagation of the flame front, the mixture within the mean flame brush tends to the local and instantaneous thermodynamic equilibrium. Based on this assumption, a method based on the sub-grid scale unburned/burnt volumes of the flame-containing cells was proposed by Liang and Reitz [15] for calculating the species conversion rate and the associated primary heat release rate. A detailed discussion of this method is given in Refs. [15,16,17]. However this model does not consider the potential heat release in the unburned region of a flame-containing cell. In the present study, we consider the heat release as follows. As shown in figure 1, we divide the flame-containing cell into three regions for the next time step  $\Delta t$ : the to be swept region ①, the

unburned region ②, and the burnt region ③. In figure 1,  $V_u$  is the unburned volume calculated in the previous time step,  $V_b$  is the burnt volume calculated in the previous time step, and  $V$  is the turbulent flame speed. The volume of region ① is:  $V_{①}=V_{sweep}$ . The volume of region ② is:  $V_{②}=V_u-V_{①}$ . The volume of region ③ is:  $V_{③}=V_b$ .

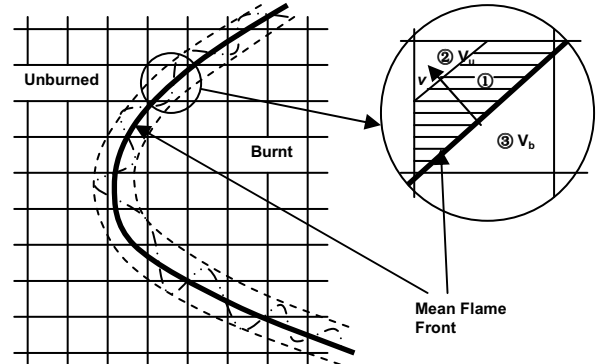


**Figure 1** Description of the turbulent flame structure

When the flame sweeps through the unburned gas region in a flame front cell (shaded region shown in figure 2) this region reaches chemical equilibrium rapidly, and it is required to determine how best to solve for the mass fraction and temperature after equilibrium. The direct way is to apply a chemical equilibrium solver to this swept region. However, the difficulty is that the initial mass fraction of this region is unknown. After the KIVA-CFD calculation, only overall parameters, such as the mass fraction of the whole cell, are known. This mass fraction is taken as the local mass fraction in the swept and burnt regions, and the temperature is taken as the temperature of the swept and burnt regions.

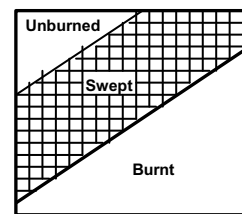


**Figure 2** Sub-grid scale unburned/burnt regions

##### (2) Model improvement

It is necessary to calculate  $d\rho_k/dt$ , where  $\rho_k$  is the density of species, "k". This can be done in several ways.

(i) The species density change rate  $d\rho_k/dt$  can be calculated with the following steps:

$$\textcircled{1} \quad \rho_b = \frac{P_{i4} W_{mix,b}}{R_u T_b} \quad (5)$$



where  $\rho_b$  is the burned region density,  $P_{i4}$  is the cell pressure,  $W_{mix,b}$  is the molecular weight of the burned mixture,  $R_u$  is the universal gas constant, and  $T_b$  is the burned mixture temperature. So the density of species "k"  $\rho_{k,b}$  in the burned region is:

$$\rho_{k,b} = \rho_b Y_{k,b} \quad (6)$$

where  $Y_{k,b}$  is the mass fraction of species "k" in the burned region.

$$\textcircled{2} \quad \rho_{k,u} = \frac{\rho_k V_{i4} - \rho_{kb} V_b}{V_u} \quad (7)$$

where  $\rho_{k,u}$  is the density of species "k" in the unburned region,  $\rho_k$  is the density of species "k" in the whole cell, and  $V_{i4}$  is the cell volume. Equation (7) assumes the mass fraction of species "k" is conserved in the cell. However this assumption is not correct because chemical equilibrium reactions transform species to other species. Hence the calculation is modified as follows ("'" indicates the new modified step):

Assume that the mass fraction in the unburned region does not change temporarily, i.e.,

$$\textcircled{2}' \quad Y_{k,u} = ck(isp) \times W_{isp} \quad (8)$$

where  $Y_{k,u}$  is the mass fraction of species "k" in the unburned region, "ck(isp)" is the mole number of species "isp" which is included in the chemical equilibrium computation before equilibrium, and  $W_{isp}$  is the molecular weight of species "isp".

$$\textcircled{3}' \quad \rho_u = \frac{\rho_{i4} V_{i4} - \rho_b V_b}{V_u} \quad (9)$$

where  $\rho_u$  is the unburned region density,  $\rho_{i4}$  is the cell density.

$$\textcircled{4}' \quad \rho_{k,u} = \rho_u Y_{k,u} \quad (10)$$

$$\textcircled{5}' \quad \frac{d\rho_k}{dt} = \rho_u (Y_{k,b} - Y_{k,u}) \frac{A_{f,i4}}{V_{i4}} S_T \quad (11)$$

where  $A_{f,i4}$  is the flame front surface area in cell "i4", and  $S_T$  is the turbulence velocity.

With  $\frac{d\rho_k}{dt}$  based on the whole cell, the specific internal energy change  $\Delta Sie$  based on the whole cell can be calculated.

(ii) A second method to calculate  $d\rho_k / dt$  is as follows.

Assume that in the time step "dt" the flame propagates through the total  $V_u$  volume, then the end density of species "k" is  $\rho Y_{k,b}$ , where  $\rho$  is the cell density. The initial density is  $\rho_k$ . So the density change rate of species "k" is:

$$\frac{d\rho_k}{dt} = \frac{\rho Y_{k,b} - \rho_k}{dt} \quad (12)$$

But this density change rate only corresponds to the volume  $V_u$ . If the actual volume  $V_s$  is swept, then the density change rate should be:

$$\frac{d\rho_k}{dt} = \left( \frac{\rho Y_{k,b} - \rho_k}{dt} \right) \frac{V_s}{V_u} \quad (13)$$

With  $\frac{d\rho_k}{dt}$  based on the whole cell, the specific internal energy change  $\Delta Sie$  is also based on the heat release in the whole cell.

(iii) The previous methods both have shortcomings and were improved as follows.

① In both methods 1 and 2 above, the model does not consider the species density change and heat release in region ②, as shown in figure 1.

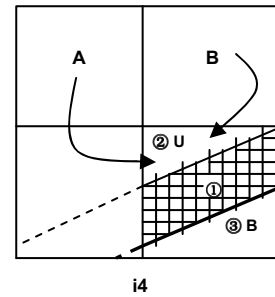


**Figure 3** Calculation of unburned region ②

However, the specific internal energy change of region ②  $\Delta Sie_2$  can be estimated as follows:

$$\Delta Sie_2 = \frac{\Delta Sie_A \rho_A V_A + \Delta Sie_B \rho_B V_B}{\rho_A V_A + \rho_B V_B} \quad (14)$$

where  $\Delta Sie_A$  and  $\Delta Sie_B$  are the specific internal energy change of unburned neighbor cells A and B, respectively, and  $\rho_A$ ,  $\rho_B$ ,  $V_A$ ,  $V_B$  are the corresponding cell density and cell volume of A and B, respectively. The species density change rate of region ②  $\left( \frac{d\rho_k}{dt} \right)_2$  is computed as

follows:

$$\left( \frac{d\rho_k}{dt} \right)_2 = \frac{\left( \frac{d\rho_k}{dt} \right)_A V_A + \left( \frac{d\rho_k}{dt} \right)_B V_B}{V_A + V_B} \quad (15)$$

where  $\left( \frac{d\rho_k}{dt} \right)_A$  and  $\left( \frac{d\rho_k}{dt} \right)_B$  are the species density change rate of cell A and B, respectively.

② In method 2, the current model considers the species density change and heat release in region ③, as shown in figure 1. However, the species density change and heat release in region ③ is not considered.

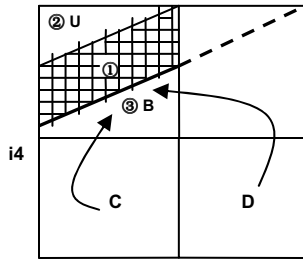


**Figure 4** Calculation of burnt region ③

In this case the average species density of the burnt neighbor cells of the current flame front cell is taken as the initial species density of region ③. For example, for two burnt neighbor cells C and D, the species densities initially are  $\rho_{kC}$  and  $\rho_{kD}$ . Then the initial species density of region ③  $\rho_{k0}$  is:

$$\rho_{k0} = \frac{\rho_{kC}V_C + \rho_{kD}V_D}{V_C + V_D} \quad (16)$$

where  $V_C$ ,  $V_D$  are the cell volumes of C and D, respectively. The species density change rate of region ③  $\left(\frac{d\rho_k}{dt}\right)_3$  is calculated as:

$$\left(\frac{d\rho_k}{dt}\right)_3 = \frac{\rho_{k,b} - \rho_{k0}}{\Delta t} \quad (17)$$

and the specific internal energy change of region ③  $\Delta Sie_3$  is:

$$\Delta Sie_3 = -\sum_k \left[ \left(\frac{d\rho_k}{dt}\right)_3 h_{fk} / (W_k \cdot \rho_b) \cdot \Delta t \right] \quad (18)$$

where  $h_{fk}$  is the heat of formation of species "k", and  $W_k$  is the molecular weight of species "k".

③ Finally, in the improved model the species density change rate  $\left(\frac{d\rho_k}{dt}\right)_{i4}$  and heat release  $\Delta Sie_{i4}$  in the cell are computed as follows:

For method 1:

$$\left(\frac{d\rho_k}{dt}\right)_{i4} = \frac{d\rho_k}{dt} + \frac{\left(\frac{d\rho_k}{dt}\right)_2 (V_u - V_{swept}) + \left(\frac{d\rho_k}{dt}\right)_3 V_b}{V_{i4}} \quad (19)$$

$$\Delta Sie_{i4} = \Delta Sie + \frac{[\Delta Sie]_2 \times \rho_u (V_u - V_{swept}) + \Delta Sie_3 \times \rho_b V_b}{\rho_{i4} V_{i4}} \quad (20)$$

For method 2:

$$\left(\frac{d\rho_k}{dt}\right)_{i4} = \frac{d\rho_k}{dt} + \frac{\left(\frac{d\rho_k}{dt}\right)_2 (V_u - V_{swept})}{V_{i4}} \quad (21)$$

$$\Delta Sie_{i4} = \Delta Sie + \frac{\Delta Sie_2 \times \rho_u (V_u - V_{swept})}{\rho_{i4} V_{i4}} \quad (22)$$

Method 2 was used in the present CFD simulations. Further improvement to the above model has also been performed. This improvement is that the chemical equilibrium solver is only applied to the shaded region, not to the whole cell. To get the initial mass fraction of species in this region, since it belongs to the unburned region the value from the unburned neighbor cells of the current flame-containing cell is taken as the initial value of this shaded region. Then the chemical equilibrium solver is called to get the chemical equilibrium species mass fraction and equilibrium temperature for this swept region. Then  $\frac{d\rho_k}{dt}$  and  $\Delta Sie$  of this swept region is

calculated. For the calculation of the unburned small region and burnt small region, CHEMKIN is used. The same process as (2)→(iii)→① is used to calculate  $\Delta Sie_2$  and  $\left(\frac{d\rho_k}{dt}\right)_2$ , and a similar process as (2)→(iii)→① is used to calculate  $\Delta Sie_3$  and  $\left(\frac{d\rho_k}{dt}\right)_3$ .

## FLAME FRONT QUENCHING MODEL

Local flame front quenching in a highly stratified charge is one of the main reasons for the relatively high unburned hydrocarbon (UHC) emissions in GTDI engines. In the present combustion model, local flame front quenching is modeled based on the turbulent combustion regime. If the local laminar flame inner layer thickness  $l_\delta$  is large enough so that the inner layer can be disturbed by the Kolmogorov eddies, chemical reactions in the inner layer will cease due to excess heat conducted out of the flame and active species loss to the preheat zone, resulting in local flame front quenching. A comparison between the inner layer thickness  $l_\delta$  and the Kolmogorov length scale  $l_K$  is used in the present study as the criterion for local flame front quenching. Flame front quenching occurs when the relation

$$l_K < c_{m3} l_\delta = c_{m3} \delta_F \quad (23)$$

is satisfied, where  $l_K$  is determined by [Ref. 7]

$$l_K = R_e^{-3/4} l_I \quad (24)$$

with the turbulent Reynolds number defined as

$$R_e = \frac{u' l_I}{S_L l_F} \quad (25)$$

and  $S_L$  is the laminar flame speed,  $l_I$  is the turbulence integral length scale obtained from the  $k-\varepsilon$  turbulence model, and  $l_F$  is the flame thickness, which can be estimated by [Ref. 15]

$$l_F = \frac{(\lambda/c_p)_{T_0}}{\rho_u S_L} \quad (26)$$

where  $\lambda/c_p$  is evaluated at inner layer temperature  $T_0$ ,

$\rho_u$  is the density of the unburned mixture. In the present model  $\delta = 0.1$ , and a tunable model constant  $c_{m3}$  is introduced.

## DAMKOHLE MODEL FOR FLAME-CONTAINING CELLS

In the previous G-equation combustion model with detailed chemical kinetics [15,16,17], once a flame front cell is identified, the G-equation flame propagation method in which the chemical equilibrium solver is applied, is used for the calculation of species density change and energy release, and CHEMKIN is used in front of and behind the flame-containing cells. In this paper, a new criterion is used to choose between the CHEMKIN and G-equation models in the flame front region [26]. A Damkohler number is introduced that is the ratio between the laminar flame propagation timescale and a chemical timescale. The time scales are used to evaluate, for every computational cell in the flame front region, whether combustion is locally controlled by flame propagation or by volumetric heat release. The Damkohler equation is defined as

$$Damk = \frac{\tau_{lam}}{\tau_{chem}} \quad (27)$$

where

$$\tau_{lam} = \frac{D_l}{S_l^2} = \frac{\delta_l}{S_l} \quad \text{and} \quad \tau_{chem} = \frac{[Fuel]}{d[Fuel]/dt} \quad (28)$$

and  $D_l$  is the laminar diffusivity,  $S_l$  is the laminar flame speed,  $\delta_l$  is the laminar flame thickness, and  $[Fuel]$  is the effective fuel concentration. Note that the use of the laminar time scale (based on the laminar flame speed and diffusivity) is consistent with the interpretation that at a subgrid level flamelets control the combustion rate. In the case that flame propagation is dominant (bigger chemical timescale) the G-equation model is used for the combustion calculation in that cell. Otherwise (bigger laminar timescale) CHEMKIN is adopted to compute the combustion rate and energy release.

## MODELING THE EFFECT OF LOCAL RESIDUAL ON BURNING VELOCITY

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

$$S_L^0 = S_{L,ref}^0 \left( \frac{T_u}{T_{u,ref}} \right)^\alpha \left( \frac{p}{p_{ref}} \right)^\beta F_{dil} \quad (29)$$

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  $\alpha$  and  $\beta$  are correlated as functions of equivalence ratio.  $F_{dil}$  is a factor that accounts for the presence of diluents, which can be expressed as:

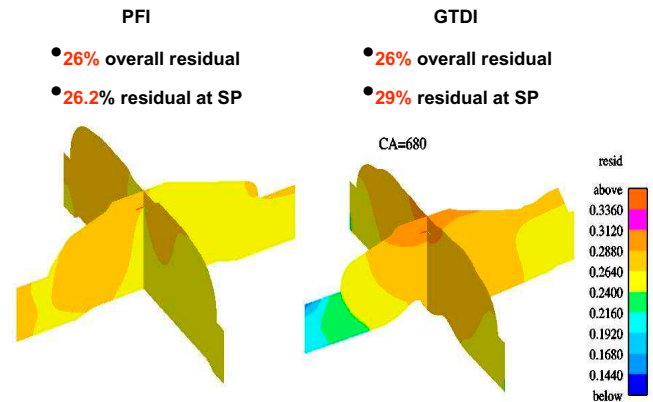
$$F_{dil} = 1 - f_{dil} Y_{dil} \quad (30)$$

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"  $Y_{dil}$

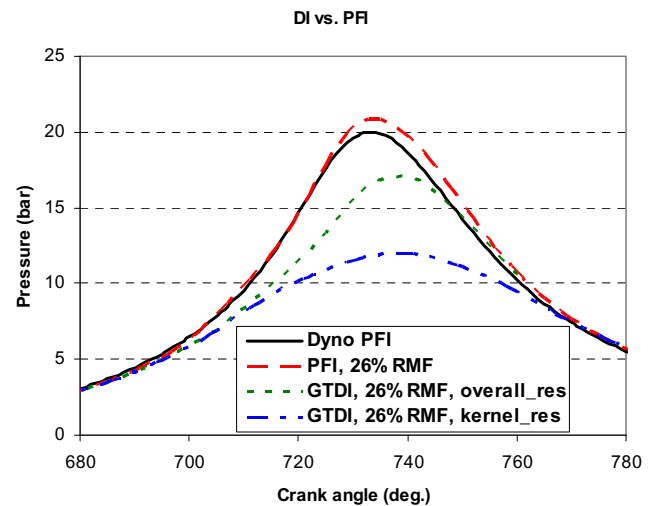
increases and the evaluation of turbulent flame speed is sensitive to the "residual mass fraction".

The 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 local residual value on burning velocity is shown in figure 5. 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