A Transport Equation Residual Model Incorporating a Damkohler Criterion for Predicting the Flame Propagation in Gasoline Direct Injection Engines

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A transport equation residual model incorporating a Damkohler criterion has been developed and implemented in the ERC KIVA-3V 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$_2$O 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$_2$O from the previous engine cycle or EGR and which is from the combustion products of the current engine cycle. In addition 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 is introduced. The criterion is based on a comparison between a laminar flame propagation time scale and the chemical kinetics time scale. 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.

1 Introduction

The combustion process in Spark-Ignition (SI) engines is a complicated aero-thermo-chemical process especially due to the fact that the turbulence and chemistry interactions occur on tremendously different time-scale and length-scale levels. The level set method is a powerful tool for describing the flame interface evolution. With its application to combustion, Williams [1] first suggested a transport equation of a non-reactive scalar, $G$, for laminar flame propagation. Peters [2] [3] 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. [4], Tan [5] [6] and Ewald et al. [7]. To better understand the fundamental engine combustion process and to further improve the versatility of multidimensional models, Liang [8] [9] [10] has incorporated detailed chemical kinetics into the $G$-equation-based turbulent combustion model which was implemented into the ERC KIVA-3V code by Tan et al. [5] [6].

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. [11] used several different methods. In this paper, we present a transport equation residual model incorporating a Damkohler criterion 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. Also, to fundamentally determine the combustion processes in flame-containing cells, a Damkohler criterion is used, in which a comparison between a laminar flame propagation time scale and a chemical kinetics time scale determining whether the $G$-equation model or chemical kinetics will be used. Finally, we present simulation results of the integrated model applied to model the combustion process in a Gasoline Turbocharged Direct Injection (GTDI) engine.

2 Model Development

2.1 $G$-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 ERC KIVA-3V code by Tan and Reitz [5] [6]. Subsequently, consideration of detailed chemical kinetics was incorporated to model the post-flame chemistry and end-gas auto-ignition chemistry by Liang and Reitz [8] [9] [10]. The $G$-equation combustion model is mainly based on the turbulent premixed
The laminar flame speed correlation used is [Ref. 8]:

\[ S_{L}^{0} = S_{L,ref}^{0} \left( \frac{T_{u}}{T_{u,ref}} \right)^{\alpha \rho} \left( \frac{p}{p_{ref}} \right)^{\beta} F_{dl} \]  

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. \( F_{dl} \) is a factor that accounts for the presence of diluents, which can be expressed as:

\[ F_{dl} = 1 - f_{dl} Y_{dl} \]  

where \( f_{dl} \) is an experimentally determined constant, and \( Y_{dl} \) is the "residual mass fraction", including CO\(_2\), H\(_2\)O and residual N\(_2\). From the above correlations, it is seen that the turbulent flame speed \( S_{T}^{0} \) decreases as the "residual mass fraction" \( Y_{dl} \) increases and the evaluation of turbulent flame speed is sensitive to the "residual mass fraction".

Yang et al. [11] 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, using the overall residual value of the cylinder, using the stored local residual mass fraction for each cell in the combustion chamber before spark ignition. They also tried to use a local and instantaneous residual formulation which can be expressed as follows:
\[ Y_{ao} = y_{co_2} (1 + 0.7273 \times 3.29 \times \alpha / 14.7) + y_{h_2o} (1 + 0.8889 \times 3.29 \times \alpha / 14.7) \] (7)

where \( y_{co_2} \) and \( y_{h_2o} \) are the mass fraction of \( \text{CO}_2 \) and \( \text{H}_2\text{O} \) respectively, and \( \alpha \) is the local air fuel ratio.

Unfortunately the results showed that these methods were limited. 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.

### 2.2.1 Computational region has no flame

![Figure 1: Computational region has no flame.](image1)

Figure 1 shows a problem in which the computational flow region has no flame propagation. Take one cell as an example. In this cell, without loss of generality, let us consider one species, e.g., \( \text{CO}_2 \). The change of the density \( \rho_{\text{CO}_2} \) of \( \text{CO}_2 \) is due to three parts: ① diffusion, denoted by “\( \vec{\nabla} \)”; ② convection, denoted by the “wave curve with arrow”; ③ chemical kinetics reaction, denoted by “\( \emptyset \)”. The initial amount of \( \text{CO}_2 \) can be assigned at the beginning of calculation. So the governing equation of the density \( \rho_{\text{CO}_2} \) of \( \text{CO}_2 \) is:

\[
\frac{\partial \rho_{\text{CO}_2}}{\partial t} + \nabla \cdot \left( \rho_{\text{CO}_2} \vec{u} \right) = \nabla \cdot \left( \rho D \nabla \rho_{\text{CO}_2} \right) + \left( \dot{\rho}_{\text{CO}_2} \right)_{\text{ChemK}}
\] (8)

### 2.2.2 Computational region has a flame

![Figure 2: Computational region has a flame.](image2)

Figure 2: Computational region has a flame.

As shown in Fig.2, consider one species, e.g., \( \text{CO}_2 \). The change of the density \( \rho_{\text{CO}_2} \) of \( \text{CO}_2 \) is still due to three parts (similar to section 2.2.1): ① diffusion, denoted by “\( \vec{\nabla} \)”; ② convection, denoted by the “wave curve with arrow”; ③ chemical reaction (including three parts: unburned side chemical kinetics reaction,
burned side chemical kinetics reaction, and the flame swept region chemical equilibrium reaction), denoted by \( \varnothing \). The initial amount of CO\(_2\) can be assigned at the beginning of calculation. So the governing equation of the density (\( \rho_{\text{CO}_2} \)) of CO\(_2\) is:

\[
\frac{\partial \rho_{\text{CO}_2}}{\partial t} + \nabla \cdot (\rho_{\text{CO}_2} \vec{u}) = \nabla \left[ \rho D \nabla \rho_{\text{CO}_2} \right] + (\dot{\rho}_{\text{CO}_2})_{\text{Chem}} \tag{9}
\]

where the calculation of \( (\dot{\rho}_{\text{CO}_2})_{\text{Chem}} \) is different from that of \( (\dot{\rho}_{\text{CO}_2})_{\text{ChemK}} \) in equation (8).

In the KIVA code equation (9) is used to calculate each species. So the \( \rho_{\text{CO}_2} \) is the density of the total CO\(_2\) in this cell. Yang et al. [11] used this \( \rho_{\text{CO}_2} \) to calculate the “residual mass fraction”, as shown in equation (7), however, this method was shown to be ineffective because the \( \rho_{\text{CO}_2} \) is not the real residual.

\[\text{Figure 3: Separate consideration of the residual part from the total amount of one species.}\]

As shown in Fig.3, CO\(_2\) is composed of two parts: one part from the residual CO\(_2\), denoted by “\( \varnothing \)”; and another part from the combustion products CO\(_2\), denoted by “\( \varnothing \). The change of the density (\( \rho_{\text{CO}_2R} \)) of the residual CO\(_2\), is due to three parts: ① diffusion, denoted by the dashed “\( \varnothing \)”; ② convection, denoted by the dashed “wave curve with arrow”; ③ chemical kinetics reaction, denoted by “\( \varnothing \). Also the change of the density (\( \rho_{\text{CO}_2C} \)) of combustion products CO\(_2\), is due to three parts: ① diffusion, denoted by the solid “\( \varnothing \)”; ② convection, denoted by the solid “wave curve with arrow”; ③ chemical reaction, denoted by “\( \varnothing \).” However, it is not required to calculate \( \rho_{\text{CO}_2C} \), because the density \( \rho_{\text{CO}_2} \) of the total CO\(_2\) species is known from Eq. (9).

Thus, we only need to focus on the calculation of the residual \( \rho_{\text{CO}_2R} \). The initial amount of residual CO\(_2\) actually is the assigned value at intake valve closure or at the beginning of the calculation. So the governing equation of the density \( \rho_{\text{CO}_2R} \) of the residual CO\(_2\) is:

\[
\frac{\partial \rho_{\text{CO}_2R}}{\partial t} + \nabla \cdot (\rho_{\text{CO}_2R} \vec{u}) = \nabla \left[ \rho D \nabla \rho_{\text{CO}_2R} \right] + (\dot{\rho}_{\text{CO}_2R})_{\text{ChemK}} \tag{10}
\]

where the calculation of \( (\dot{\rho}_{\text{CO}_2R})_{\text{ChemK}} \) will be described later.

In reality there are other residual species. If we have \( N \) residual species, then we can sum Eq. (10) from \( i=1 \) to \( N \).

\[
\sum_{i=1}^{N} \left[ \frac{\partial \rho_{\text{ir}}}{\partial t} + \nabla \cdot (\rho_{\text{ir}} \vec{u}) \right] = \nabla \left[ \rho D \nabla \rho_{\text{ir}} \right] + (\dot{\rho}_{\text{ir}})_{\text{ChemK}}
\]

\[
\Rightarrow \quad \frac{\partial \rho}{\partial t} + \nabla \cdot \left( \rho \vec{u} \right) = \nabla \left[ \rho D \nabla \rho \right] + \sum_{i=1}^{N} (\dot{\rho}_{\text{ir}})_{\text{ChemK}}
\]

Defining a “pseudo” species, named “Ar”, which is the \( \sum_{i=1}^{N} \rho_{\text{ir}} \), and writing \( \sum_{i=1}^{N} (\dot{\rho}_{\text{ir}})_{\text{ChemK}} \) as \( (\dot{\rho}_{\text{Ar}})_{\text{ChemK}} \), the above equation becomes
\[ \frac{\partial \rho_{Ar}}{\partial t} + \nabla \cdot (\rho_{Ar} \vec{u}) = \nabla \cdot [\rho D_{Ar} \nabla \rho_{Ar}] + (\rho_{Ar})_{ChemK} \]  \hspace{1cm} (11)

Equation (11) is the final residual transport equation. To calculate \((\dot{\rho}_{Ar})_{ChemK}\), \((\dot{\rho}_{R})_{ChemK}\) of each species is calculated separately, then \((\dot{\rho}_{Ar})_{ChemK}\) is the summation of \((\dot{\rho}_{R})_{ChemK}\) of all residual species. The initial amount of the “pseudo” species “Ar” actually is the summation of the assigned value of each residual species at the beginning of the calculation, or can be calculated from Eq. (7).

To solve the residual transport Eq. (11), \(\nabla \cdot [\rho D_{Ar} \nabla \rho_{Ar}]\) can be calculated in the species mass fraction iteration subroutine (in KIVA: “yit-transp.f”), and \(\nabla \cdot (\rho_{Ar} \vec{u})\) can be calculated in the advection flux calculation subroutine (in KIVA: “ccflux-transp.f”). As mentioned earlier, \((\dot{\rho}_{Ar})_{ChemK}\) is the summation of \((\dot{\rho}_{R})_{ChemK}\) of all residual species. For the calculation of \((\dot{\rho}_{R})_{ChemK}\) CHEMKIN is called to calculate \((\dot{\rho}_{i})_{ChemK}\) for each cell “i” and because \((\dot{\rho}_{i})_{ChemK} = (\dot{\rho}_{R})_{ChemK} + (\dot{\rho}_{NotR})_{ChemK}\), we have

\[
(\dot{\rho}_{Ar})_{ChemK} = (\dot{\rho}_{i})_{ChemK} \times \frac{\rho_{Ar}}{\rho_{i4}}.
\]

It should be noticed that the equation of state is still \(P = R_a T \sum_{i=1}^{nsp} \left( \frac{\rho_i}{W_i} \right)\), where “nsp” excludes the fictitious species “Ar”, because the \(\rho_i\) is already the density of the all “i” species, which includes the residual part of the species “i”. It should also be noticed that in both the species mass fraction iteration subroutine and the flux calculation subroutine, the diffusion and convection of the “pseudo” species “Ar” do not contribute to the mass and enthalpy change of the computed cell, because the diffusion and convection are already calculated for each species “i”.

After solving the residual transport equation, the “residual mass fraction” can be calculated as \(Y_{dit} = \rho_{Ar}/\rho_{i4}\) in each computational cell.

### 2.3 Damkohler number criterion for combustion regime in flame containing cells

In previous implementations of the G-equation combustion model with detailed chemical kinetics [8] [9] [10], 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 [13]. A Damkohler number is introduced that is the ratio between the laminar flame propagation timescale and a chemical timescale. These time scales are used to evaluate, for every computational cell in the flame front region, whether combustion is locally controlled by flame propagation (e.g., flamelets) or by volumetric heat release. The Damkohler equation is defined as

\[
Damk = \frac{\tau_{lam}}{\tau_{chem}}
\]

where

\[
\tau_{lam} = \frac{D_i}{S_f} = \delta_i S_i \quad \text{and} \quad \tau_{chem} = \frac{[Fuel]}{d[Fuel]/dt}
\]

and \(D_i\) is the laminar diffusivity, \(S_f\) is the laminar flame speed, \(\delta_i\) is the laminar flame thickness, and \([Fuel]\) is the effective fuel concentration (i.e., fuel+CO+H\textsubscript{2} species). 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 flame timescale) CHEMKIN is adopted to compute the combustion rate and energy release.

### 3 Model Validation

The engine studied is a Gasoline Turbocharged Direct Injection (GTDI) engine operated at two conditions. One operating condition is a high load uniform mixture case (2000 rev/min, boosted charge), and the other one is low load uniform mixture case (1500 rev/min). The specifications of the engine and the modeled operating conditions are listed in Table 1.
Table 1: Specifications and operating conditions of the studied engine [11].

<table>
<thead>
<tr>
<th>Operating Conditions</th>
<th>High load</th>
<th>Low load</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore / Stroke</td>
<td>92.5 mm / 86.7 mm</td>
<td></td>
</tr>
<tr>
<td>Connecting Rod Length</td>
<td>152.4 mm</td>
<td></td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>9.7</td>
<td>10.09</td>
</tr>
<tr>
<td>Engine Speed</td>
<td>2000 rev/min</td>
<td>1500 rev/min</td>
</tr>
<tr>
<td>Spark Timing (° ATDC)</td>
<td>-11</td>
<td>-37</td>
</tr>
<tr>
<td>Overall Residual</td>
<td>2%</td>
<td>25%</td>
</tr>
<tr>
<td>MAP</td>
<td>165.3 kPa</td>
<td>55.24 kPa</td>
</tr>
<tr>
<td>End-of-Injection (° ATDC)</td>
<td>201.37</td>
<td>-286.3964</td>
</tr>
</tbody>
</table>

Figure 4: Computational mesh of the Gasoline Turbocharged Direct Injection engine at -50° CA ATDC.

The computational mesh contains around 190,000 cells, including the intake and exhaust manifolds and the cylinder, as can be seen in Figure 4. A reduced 25-species, 51-reaction iso-octane mechanism [14] including the NOx reactions was used to model the post-flame chemistry and the low temperature chemistry in the end gas. CHEMKIN II was used to solve the detailed chemical kinetic equations.

3.1 Results from the transport equation residual model

Figure 5 shows the overall residual mass fraction of the cylinder and the average residual of the flame front cells for the high load uniform mixture case (2000 rev/min, boosted charge) (note that the flame front is not defined before the time of ignition). From figure 5 it is seen that the overall residual has a slight change, but the residual at the flame front cells has some changes around the overall residual value. The changing residual value at the flame front cells affects the laminar flame speed locally. Figures 6(a,b) show a comparison between the species “Ar” mass fraction distribution and the total local “residual” distribution. From figure 6 it is seen that the residual at the flame front cells from the transport equation model is around 1.7%, which is close to the overall residual of the engine at high load operating condition and thus the residual from the transport equation is considered as the local, instantaneous and accurate residual value, while the total local residual value at the flame front is about 20%, which can not correctly represent the real residual value. That is the reason why directly using the “local residual formulation” method mentioned earlier was ineffective.
3.2 Results from the Damköhler criterion model

Figures 7(a,b,c) show the pressure comparison between the $G$-equation model (flame propagation) and the CHEMKIN model (volumetric heat release) and the use of the Damköhler number criterion of Eq.12 with different critical Damköhler numbers, for the GTDI engine high load uniform mixture case (2000 rev/min, boosted charge), the GTDI low load uniform mixture case (1500 rev/min), and a GTDI low load highly stratified mixture case (1500 rev/min). As expected, from Figure 7 it is seen that the results from the Damköhler model lie between the $G$-equation model and the pure CHEMKIN case. For premixed charge engine cases flame propagation dominates, so the pure CHEMKIN gives poor results. As the Damköhler number increases, the results approach the pure $G$-equation model. Note that the combustion model constants used in the present computation correspond to those of Liang et al. [8] [9] [10], and would need to be revised if the Damköhler criterion is adapted.

(a) GTDI engine high load uniform mixture case
3.3 Results for high and low load operation

Figures 8(a,b,c,d) show the final calibration results of the low load uniform mixture case (1500 rev/min) after using the transport equation residual model incorporating the Damkohler criterion. In this calibration the set of combustion parameters is: $cm4 = 0.7$ where $cm4$ is the spark kernel to $G$-model transition model constant [8], and Damkohler number $= 1.0$. From the results it is seen that the simulation results match the experimental results very well.
4 Conclusions

A transport equation residual model incorporating a Damkohler number criterion has been developed and implemented in the ERC KIVA-3V code. The advantage of the transport equation residual model is that it differentiates CO\(_2\) and H\(_2\)O from the previous engine cycle or EGR from the combustion products of the current engine cycle. Thus the model accurately traces the local and instantaneous residual values in the flame front cells, which have a great effect on the laminar flame speed. The Damkohler criterion fundamentally determines whether the \(G\)-equation model or chemical kinetics should be used for assessing the combustion processes in the
flame-containing cells based on the comparison between the laminar flame propagation timescale and the chemical kinetics timescale. 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 operational conditions, good agreement with experimental in-cylinder pressure, heat release rates and Mass Fraction Burned (MFB) data was obtained.

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References