State of the Art of Modeling of Combustion and pollutants in Spark Ignited Engine

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INTRODUCTION: Some key factors for modeling

1. Downzoning (fuel efficiency)
2. Gas exchange
3. Mixture preparation
   ✓ Spray, Droplets wall interaction
   ✓ Liquid film
4. Spark
5. Main flame propagation
   ✓ Laminar flame properties: speed, thickness
   ✓ Mean and turbulent propagation
6. Wall heat transfer
7. Kinetics for Auto-Ignition (knock)
8. Emissions
INTRODUCTION

1D code are well established for engine components design

But they still need **input parameters from combustion** (and other physics,...)

The combustion approximated by 0D model rely on Wiebe function

- Burning Rate
- Combustion Efficiency
- Spray, mixing,
- Spark, combustion,

Needs for predictive and accurate 3D models
Recent progress is attributed to the development of models which explicitly take into account the fact that combustion occurs in the wrinkled or corrugated flame regime (or broken reaction zone).

- Coherent Flame Model (CFM-ITNFS)
- Weller 1 equation Flame Wrinkling model
- Weller 3 equations model
- ECFM-3Z / ECFM-CLEH
- **G-equation Level set Model**
Introduction: Schematic of Premixed Regimes

Flame brush is thickened
Flame structure changes

Engine flames*
& Level set field

Karlolwitz > 1
Laminar flame thickness > smallest turbulent scale

Karlolwitz < 1
Laminar flame thickness > smallest turbulent scale

* Peters, Reitz
G-equation - Model concept *

- Introduce $n$ as vector normal to front flame:

\[ n = -\frac{\nabla G}{|\nabla G|} \]

- The flow field propagation:

- Thus the sum of flow velocity and burning velocity in normal direction:

\[ \frac{dx_f}{dt} = v_f + n s_L \]

- A field of $G$ can now be calculated:

\[ \frac{\partial G}{\partial t} + \nabla G \cdot \frac{dx_f}{dt} = 0 \]

*N.Peters, H.Pitsh*
G-equation or Level set approach

- G-equation determines flame location in spark-ignition/main combustion stages

  • The non-reacting scalar $G$ locate the Flame Front

  $\frac{\partial G}{\partial t} + \vec{U} \cdot \nabla G = S_t |\nabla G| - D_T \vec{k} \cdot \nabla \vec{G}$

Curvature term: Usually small and neglected *

The above equation avoids complications with counter-gradient diffusion, and since $G$ is no-reacting scalar, **there is non need for a source term closure**

*Reitz
Turbulent flame structure

Ensemble averaged flamelets

\[
\frac{\partial G}{\partial t} + \bar{U} \cdot \nabla G = S_t |\nabla G|
\]

Due to the increased surface area, turbulent flame brush propagates at enhanced velocity

\[
\frac{\partial}{\partial t} \rho G' + \frac{\partial}{\partial x_i} \rho u_i G' - \rho s_T \frac{\nabla G' \cdot \nabla G}{|\nabla G|} = 2 \frac{\mu_i}{\sigma_i} \left[ \frac{\partial G}{\partial x_i} \frac{\partial G}{\partial x_i} \right] - c_s \rho \frac{\varepsilon}{k} G'
\]

G' variance from which we can obtain flame thickness

\[
c = a_3 \left[ \text{erf} \left( a_1 G/l_{F,t} - a_2 \right) + 1 \right]
\]
Additional equations for mixture inhomogeneity

\[
\frac{\partial}{\partial t} \rho Z + \frac{\partial}{\partial x_i} \rho u_i Z = \frac{\partial}{\partial x_i} \left[ \left( D_z \rho + \frac{\mu_i}{\sigma_i} \right) \frac{\partial Z}{\partial x_i} \right]
\]

\[
\frac{\partial}{\partial t} \rho Z' + \frac{\partial}{\partial x_i} \rho u_i Z' - \frac{\partial}{\partial x_i} \left[ \left( D_z \rho + \frac{\mu_i}{\sigma_i} \right) \frac{\partial Z'}{\partial x_i} \right]
= 2 \frac{\mu_i}{\sigma_i} \left[ \frac{\partial Z}{\partial x_i} \frac{\partial Z}{\partial x_i} \right] - c_s \rho \frac{\varepsilon}{k} Z'
\]

\[
s_T(\Phi) = s_i^0(\Phi) \left[ 1 + A \left( \frac{u'}{s_i^0(\Phi)} \right)^{5/6} \right]
\]

\[
s_T = \int_0^1 s_T(\Phi) P(Z) \, dZ
\]
POST-FLAME COMBUSTION REACTIONS

A: Laminar flame speed
B: Post-flame chemistry
C: Nox Model – NORA
D: Soot model (Sectional method)

A) Gülder correlation for Laminar Flame speed

B) 7 species Equilibrium: CO2, CO, H2O, OH, O, N, H2

C) N2O \rightarrow N2 \rightarrow NNH
   N \rightarrow NO \rightarrow HCN, NCN

D) PAH volume:
   \[ V_{PAH} = 0.3 \cdot 10^{-28} \text{ m}^3 \]

D) There are 20 (or more) sections of volume \( \Rightarrow \) 20 sections of diameter
Application I: GDI Spray Guide: Full load RPM Variation

2000 - 3000 - 5800 RPM
Application I: GDI – Spray guided – Full load RPM variation

Pressure history

**Experiment**

**Prediction**

2000 RPM

3000 RPM

5800 RPM

Apparent rate of Heat Release
CO and CO2 Levels at end of closed cycle [%]

**CO emissions:**
- **Experimental**
- **STAR-CD**

**CO2 emissions:**
- **Experimental**
- **STAR-CD**

**NOx emissions:**
- **Experimental**
- **STAR-CD**

**IMEP on closed cycle [bar]**
- **Experimental**
- **RUN**
Application II: GDI – Wall guided – High RPM Full load
Application II: GDI – Wall guided – High RPM Full load

<table>
<thead>
<tr>
<th>Configuration 1</th>
<th>Configuration 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low T.K.E</td>
<td>High T.K.E</td>
</tr>
</tbody>
</table>
Application II: GDI – Wall guided – High RPM Full load
Configuration 1/2

Pressure history

Configuration 1
Low T.K.E

Apparent rate of Heat Release

Configuration 2
High T.K.E

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Experiments
Prediction
Application II: GDI – Wall guided – High RPM Full load
Configuration 2

- From the instantaneous energy balance (including wall heat transfer):
  Get the instantaneous effective heat release

- Integrate over time the instantaneous in-cylinder chemical heat release

![Graph showing Combustion Efficiency with Mass Burnt Fraction and Inputs to 1D code](Image)

- Combustion efficiency
- 10%-90% duration
- 50% anchoring

Inputs to 1D code
SUMMARY

✓ G-equation in STAR-CD V4.26 has been investigated and validated for different engine configurations

✓ Mainly full load combustion have been investigated

✓ G-equation in STAR-CD demonstrate good capabilities under these condition (Homogeneous and GDI)

✓ Application and validation to SI-GDI (homogeneous) and PFI engines

- Good match for global thermodynamic quantities
- Good match for combustion history
- Good match for combustion history (10%-90% burn, 50% anchoring, combustion efficiency)

✓ Application to part load and validation for emissions investigations

- Link G-equation to soot sectional method – good level of soot
- Link G-equation to N.O.R.A NOx models – good match with NOX