A Computationally Efficient Combustion Progress Variable (CPV) Approach for Engine Applications

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The main target within internal combustion engine simulation is to achieve predictive results.

Detailed chemistry schemes play a key role

- to reproduce fuel sensitivities
  - Knocking combustion
  - ....
- to predict emissions
  - NOx
  - Soot
  - Unburned hydrocarbons
  - ....
- to understand new combustion concepts
  - Water injection
  - RCCI
  - ....

Objective

- Availability of detailed chemistry schemes and their complexity are increasing

Dilemma in 3D

More species lead to more accurate results, but also to a high demand of computational costs

Solution

Tabulated chemistry approaches where CPU time is independent of the number of species in the reaction mechanism

Outline

1. Objective

2. The Combustion Progress Variable (CPV) Model

3. Applications:
   - Diesel Engine
   - Spark Ignition Engine
   - CPU Times

4. Conclusions
THE COMBUSTION PROGRESS VARIABLE (CPV) MODEL
General Idea of the CPV (Combustion Progress Variable) Model

- The well-stirred reactor (WSR) combustion model is increasing again in popularity.

- The larger the mechanism is, the more species are transported, and the more CPU time is required for solving combustion chemistry.

- Idea: use $h_{298}$ as progress variable as we have before for transient flamelet models and cell local CMC for combustion, and apply to the WSR combustion model.
  - Benefit: Mechanism size will not affect CFD run-time, since all combustion chemistry is pretabulated and the number of scalars to transport will be the same regardless of chemical mechanism.
The Progress Variable

- **Idea**: A progress variable $C$ can be used for reconstruction of the thermo-chemical state on the whole reaction trajectory.
  - $C = 0$: unreacted mixture
  - $C = 1$: fully burned mixture
  - Track both low and high temperature reactions

- The fuel oxidation is parametrized using chemical enthalpy $h_{298}$

$$C = \frac{h_{298} - h_{298,0}}{h_{298,eq} - h_{298,0}}$$

$h_{298}$ current chemical enthalpy in the cell
$h_{298,0}$ enthalpy of formation at standard state (maximum)
$h_{298,eq}$ chemical enthalpy at maximum total heat release (minimum)

Chemical enthalpy and temperature as a function of time for a constant pressure calculation at 10 bar and 750 K for an n-heptane/air mixture at $\phi=1$.  

Lehtiniemi et al., Combust Sci Technol 178, 2006
Matrisciano et al., SAE Technical Paper 2017-01-05
The Chemistry Look-up Table

- Detailed chemistry scheme is solved using adiabatic constant pressure reactors
- The created table is surrogate sensitive, but independent of operating conditions as speed, engine geometry, EGR amount, load, ....
- A fully automated tool for the table generation is available: LOGEtable

### Table look-up parameters
- Pressure $p$
- Unburned Temperature $T$
- Equivalence ratio $\phi$
- EGR amount $Y_{EGR}$

### Info stored in the look-up table
- Progress variable source terms $\frac{dc}{dt}$
- Molar mass of the mixture $M_{mix}$
- Thermodynamic polynomial coefficients
- Chemical species for thermodynamics
- Any chemical species that the user decides to monitor
- Emission source terms

**Fuel**
- O$_2$
- N$_2$
- CO$_2$
- H$_2$O
- CO
- H$_2$
- C$_2$H$_2$
- C$_2$H$_4$

**Soot**
- NO$_x$
The Chemistry Look-up Table

- Exemplary dimensions of a CPV table for Diesel application

<table>
<thead>
<tr>
<th>Property</th>
<th>Range</th>
<th>Grid points</th>
</tr>
</thead>
<tbody>
<tr>
<td>EGR [%]</td>
<td>0.0 – 40.0</td>
<td>5</td>
</tr>
<tr>
<td>Equivalence ratio [-]</td>
<td>0.2 - 4.0</td>
<td>19</td>
</tr>
<tr>
<td>Pressure [bar]</td>
<td>1.0 - 200.0</td>
<td>17</td>
</tr>
<tr>
<td>Unburnt temperature [K]</td>
<td>350.0 - 1400.0</td>
<td>67</td>
</tr>
<tr>
<td>Progress Variable</td>
<td>0.0 -1.0</td>
<td>15</td>
</tr>
</tbody>
</table>

- Table generation done via LOGEtable v1.0
  - CPU time for table generation: 3h on 8 parallel cores (2016)

Temperature Grid Points:
- 3 points in the range [350 ; 550] K
- 45 points in the range [560 ;1000] K
- 11 points in the range [1020 ;1200] K
- 8 points in the range [1225 ;1400] K

191 520 points

1 GB
The combustion model is replaced, chemistry solution from the look-up table
- Transport of passives and species by CFD code
- Communication over source subroutine

**CFD Code**
- Transport of:
  - Chemical enthalpy $H_{298}$
  - Mixture fraction $Z$
  - Mass fraction EGR $Y_{EGR}$
  - Species for thermodynamics
  - Emissions
- Extra output species are assigned as passive_nt

**Combustion Progress Variable Model**
- Table look-up parameters:
  - $p$
  - $T$
  - $\phi$
  - $Y_{EGR}$
- Update of sources:
  - $H_{298}$
  - $Z$
  - $Y_{EGR}$
- Species / emission update

**Combustion**
- Well-stirred reactor model with source terms from the CPV table

**Soot**
- Method of Moments $M_0$ and $M_1$

**NOx**
- Thermal NO

2018-03-21
Additional transport equations

- **Mixture fraction**

\[
\frac{\partial \bar{ho} \bar{Z}}{\partial t} + \nabla \cdot (\bar{ho} \bar{v} \bar{Z}) - \nabla \cdot (\bar{ho} D_t \nabla \bar{Z}) = \frac{\bar{\rho} \bar{\omega}_s}{\bar{\rho}}
\]

- **Progress variable**

\[
\frac{\partial \bar{\rho} \bar{h}_{298}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{v} \bar{h}_{298}) - \nabla \cdot (\bar{\rho} D_t \nabla \bar{h}_{298}) = \frac{\bar{\rho} \bar{\omega}_s,h_{298}}{\bar{\rho}} + \frac{\bar{\rho} \bar{\omega}_{chem,h_{298}}}{\bar{\rho}}
\]

- If tuning is required, it is possible to scale the chemical reaction source term

- **CPV thermo-species (9 species)**

\[
\frac{\partial \bar{\rho} \bar{Y}_\alpha}{\partial t} + \nabla \cdot (\bar{\rho} \bar{v} \bar{Y}_\alpha) - \nabla \cdot (\bar{\rho} D_t \nabla \bar{Y}_\alpha) = \frac{\bar{\rho} \bar{\omega}_s \delta_{\alpha \beta}}{\bar{\rho}} + \frac{\bar{\rho} \bar{\omega}_\alpha}{\bar{\rho}}
\]
Additional transport equations (cont.)

- Thermal NO marker
  
  \[
  \frac{\partial (\rho \tilde{Y}_{NO})}{\partial t} + \nabla \cdot (\rho \tilde{v} \tilde{Y}_{NO}) - \nabla \cdot (\rho D_t \nabla \tilde{Y}_{NO}) = \rho \omega_{NO}
  \]

- Soot moments \( M_0 \) and \( M_1 \)
  
  \[
  \frac{\partial (\rho \tilde{M}_r)}{\partial t} + \nabla \cdot (\rho \tilde{v} \tilde{M}_r) - \nabla \cdot (\rho D_t \nabla \tilde{M}_r) = \rho \tilde{\omega}_r
  \]

- The thermal NO model can be calibrated using calibration parameters A, B, C and D. Usually it is only needed to use parameter A.

- The soot model allows for calibration through scaling source terms for:
  - Nucleation, Surface growth, fragmentation, oxidation by \( O_2 \) and oxidation by OH
APPLICATION: DIESEL ENGINE
Diesel Engine Application (1)

- **Reaction scheme**
  - Reduced n-heptane reaction scheme
    - 56 species and 206 reactions
  - Low and high temperature chemistry
  - Pathways for major engine out emissions

- **Engine case**
  - 1600 rpm
  - Single injection at 9°CA bTDC
  - EGR amount 4% and 30%
  - Bore 137mm
  - Stroke 165 mm
  - Connecting rod 263 mm

- **CPV table**

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<thead>
<tr>
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<tr>
<td>EGR [%]</td>
<td>0.0 – 50.0</td>
<td>6</td>
</tr>
<tr>
<td>Equivalence ratio [-]</td>
<td>0.1 - 10.0</td>
<td>38</td>
</tr>
<tr>
<td>Pressure [bar]</td>
<td>1.0 - 200.0</td>
<td>24</td>
</tr>
<tr>
<td>Unburnt temperature [K]</td>
<td>300.0 - 1500.0</td>
<td>89</td>
</tr>
</tbody>
</table>

Seidel et al., J. Eng. Gas Turbines and Power 2017
Diesel Engine Application (1) – Combustion Prediction

- Validation against on-line chemistry solver
  - CPV model is compared to a on-line well-stirred reactor model (LOGE API)
- EGR amount 4% and 30%
Diesel Engine Application (1) – Combustion Prediction

LOGE API – 30 % EGR

<table>
<thead>
<tr>
<th>temp [K]</th>
<th>CA: -4.99 deg</th>
<th>CA: -0.99 deg</th>
<th>CA: 3.01 deg</th>
</tr>
</thead>
<tbody>
<tr>
<td>2800.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2445.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2090.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1735.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1380.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1025.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>670.0</td>
<td>CA: 7.00 deg</td>
<td>CA: 11.01 deg</td>
<td>CA: 15.00 deg</td>
</tr>
</tbody>
</table>

CPV – 30 % EGR

<table>
<thead>
<tr>
<th>temp [K]</th>
<th>CA: -5.00 deg</th>
<th>CA: -1.00 deg</th>
<th>CA: 3.00 deg</th>
</tr>
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<tbody>
<tr>
<td>2800.0</td>
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<td>CA: 15.01 deg</td>
</tr>
</tbody>
</table>
Diesel Engine Application (2)

- **Reaction scheme**
  - LOGEDiesel:
    - Surrogate: 75% n-Decane and 25% α-Methyl-Naphthalene
    - 189 species and 2483 reactions
  - Low and high temperature chemistry
  - Pathways for major engine out emissions

- **Engine case**
  - 1600 rpm
  - Single injection at 9°CA bTDC
  - EGR amount 4%, 15% and 30%
  - Bore 137mm
  - Stroke 165 mm
  - Connecting rod 263 mm

- **CPV table**

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<thead>
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<td>Pressure [bar]</td>
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<tr>
<td>Unburnt temperature [K]</td>
<td>300.0 - 1500.0</td>
<td>22</td>
</tr>
</tbody>
</table>
Diesel Engine Application (2) – Emissions Prediction

- Soot and NO\textsubscript{x} prediction are as expected from literature
- 4\% EGR has highest soot formation and oxidation rates
- Soot-NO\textsubscript{x} trade-off is reasonable
APPLICATION: SPARK IGNITION ENGINE
Spark Ignition Engine Application

- **Reaction scheme**
  - PRF reaction scheme
    - Surrogate octane rating: 95
    - 48 species and 152 reactions
  - NO\textsubscript{x} updates
  - Pathways for major engine out emissions

- **Engine case**
  - 3000 rpm
  - Spark timing 15°CA bTDC
  - Bore 86 mm
  - Stroke 90 mm
  - Connecting rod 180 mm

- **CPV table**

<table>
<thead>
<tr>
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<th>Range</th>
<th>Grid points</th>
</tr>
</thead>
<tbody>
<tr>
<td>EGR [%]</td>
<td>0.0 – 10.0</td>
<td>3</td>
</tr>
<tr>
<td>Equivalence ratio [-]</td>
<td>0.9 – 1.1</td>
<td>5</td>
</tr>
<tr>
<td>Pressure [bar]</td>
<td>1.0 - 200.0</td>
<td>17</td>
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Yao-Dong et al. Energy and Fuels, 2012
Spark Ignition Engine – Combustion Prediction

- Validation against on-line chemistry solver
  - CPV model is compared to a online well-stirred reactor model (SAGE)
Spark Ignition Engine – Combustion Prediction

- Validation against on-line chemistry solver
## CPU Times

- All calculations are carried out on 32 cores (2008)
- Speed up factor: 2 and higher

<table>
<thead>
<tr>
<th></th>
<th>Number of Species</th>
<th>Chemistry solver</th>
<th>CPU time [hours]</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Diesel Sector Case</strong></td>
<td>56</td>
<td>On-line</td>
<td>36.7</td>
</tr>
<tr>
<td></td>
<td>56</td>
<td>LOGE-CPV</td>
<td>15.7</td>
</tr>
<tr>
<td></td>
<td>189</td>
<td>LOGE-CPV</td>
<td>15.2</td>
</tr>
<tr>
<td><strong>SI - Full Cylinder Case</strong></td>
<td>48</td>
<td>On-line</td>
<td>73.8</td>
</tr>
<tr>
<td></td>
<td>48</td>
<td>LOGE-CPV</td>
<td>40.1</td>
</tr>
</tbody>
</table>

No CPU time increase due to additional soot and NO\textsubscript{x} model or more species
CONCLUSIONS
Conclusions

- A Combustion Progress Variable (CPV) approach is presented
  - Model shows a reasonable good agreement to on-line chemistry solver
  - Model is applicable to DI and SI combustion simulation
  - Emission prediction is physical reasonable
  - CPV tables are applicable over a wide range of operating conditions

- CPU times
  - Speed up of factor 2 for the 56 species mechanism, higher speed-up for larger mechanisms (up to factor 700)
  - Emission prediction free of CPU costs

- Next steps:
  - Updates to species treatment for thermodynamics
  - Updates to improve vaporization
CONTACT

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