ANALYSIS OF A TURBOCHARGED HCCI ENGINE USING A DETAILED KINETIC MECHANISM

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Outline

• Motivation
  • Objective
    • 1-D CFD code – kinetic code interface
    • Possible uses
  • Test case
    • Different heat transfer approach
  • Conclusions
  • Future work
Motivation

Homogeneous Charge Compression Ignition

Merits

- High thermal efficiency
- Low NOx emissions
- Low soot emissions

Demerits

- Difficulties in engine control
- High HC emissions
- High CO emissions
- Low loads
Objective

Full cycle simulation tool

- Accurate evaluation of the GLOBAL ENGINE PERFORMANCES
- Accurate evaluation of the COMBUSTION PROCESS KINETIC
1-D CFD code – kinetic code interface

1-D fluid-dynamics code:

**GT-Power**
( Gamma Technologies, Inc. )

- Processes occurring in the inlet and exhaust layouts
- Injection system
- Turbocharger
- Waste-gate valve
- Intercooler
- EGR system
- Duty cycles
- Control strategies

Detailed kinetic code:

**Ignition Code**
( Lund Institute of Technology )

- Chemical reactions occurring during combustion
- Ignition delay
- Combustion heat release
- Engine emissions
1-D CFD code – kinetic code interface

Ignition Code:

Homogeneous Reactor Model

Global Quantities:

- Instantaneous Volume
  \[ V(\Theta(t)) = V_c + \frac{\pi \cdot B^2}{4} \left( 1 + a - a \cdot \cos(t^2 - a^2 \cdot \sin^2 \Theta(t))^{1/2} \right) \]

- Mean density
  \[ \rho(t) = \frac{m}{V(t)} \]

- In-cylinder pressure
  \[ p(t) = \langle \rho(t) \rangle \frac{R}{M} \left(\frac{T}{\langle M \rangle}\right) \]

Source Terms:

- Effect of chemical kinetics
  \[ Q_i = \frac{M_i}{\rho} \sum_{j=1}^{R} V_{i,j} \omega_j \quad i = 1, \ldots, S \]

- Effect of change in volume, heat losses, and reactions
  \[ Q_{S+1} = \frac{1}{c_v} \sum_{i=1}^{S} \left( h_i - \frac{RT_i}{M_i} \right) \frac{M_i}{\rho} \sum_{j=1}^{R} V_{i,j} \omega_j + p \frac{1}{c_v} \frac{dV}{dt} + \]
  \[ -\frac{1}{c_v} (h_{\text{fg}}(T - T_w) + \frac{1}{c_v} A\sigma\varepsilon (T^4 - T_w^4)) \]
1-D CFD code – kinetic code interface

Link between GT-Power and Ignition code
1-D CFD code – kinetic code interface

- Cylinder’s number, cycle’s number
- Current crank angle degree, time step size
- Current in cylinder pressure and temperature values
- Air and fuel mass trapped into the cylinder
- User parameters

At every GT-Power time step

- Ignition crank angle degree
- Burned fuel mass during the current time step
- Combustion end crank angle degree
  (In cylinder pressure and temperature values at the end of
  the current time step)

The mass fractions of the in cylinder mixture components
are stored in an external file

At every Ignition Code time step
1-D CFD code – kinetic code interface

GT-Power → User inputs → Ignition Code

Input files:
- MECOUT_80.txt
- THERMOUT80.txt
- FuelOxidizerComp.txt
Possible uses

• Evaluation of the influence of engine operating parameters on the combustion process
  (Ignition delay, combustion duration, pollutant emissions)

• Evaluation of the influence of the combustion process on engine operating parameters
  (IMEP, BSFC, exhaust gas temperature, turbocharger speed and efficiency)

• Comparison of different engine control strategies under duty cycle operating conditions
### Test case

**SCANIA DSC12**

(DI turbocharged Diesel engine)

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total displacement</td>
<td>11 705 cm³</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>18:1</td>
</tr>
<tr>
<td>Bore</td>
<td>127 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>154 mm</td>
</tr>
<tr>
<td>Connecting Rod</td>
<td>255 mm</td>
</tr>
<tr>
<td>IVO</td>
<td>54° BTCD</td>
</tr>
<tr>
<td>IVC</td>
<td>78° ABCD</td>
</tr>
<tr>
<td>EVO</td>
<td>96° BBCD</td>
</tr>
<tr>
<td>EVC</td>
<td>54° ATCD</td>
</tr>
</tbody>
</table>

**FUEL ADOPTED FOR HCCI OPERATING CONDITIONS**

- ISOOCTANE
- N-HEPTANE
Test case

iso - Octane

$1000 (K) / \text{Temperature}$

Ignition Delay Time (ms)

- Deflagration
- Detonation
- Mechanism

$\Phi = 1.0, p = 40\ \text{bar}$
Test case

$\text{n - Heptane}$
Test case

- deflagration
- detonation

PHI = 1.0, p = 40 bar

Ignition Delay Time (ms)

60% iso – Octane and 40% n - Heptane
Test case

**Model validation:**

**Operating conditions:**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>3.07</td>
</tr>
<tr>
<td>rpm</td>
<td>1500</td>
</tr>
<tr>
<td>ON</td>
<td>100</td>
</tr>
<tr>
<td>Eng. Inlet Temp. [K]</td>
<td>424</td>
</tr>
<tr>
<td>Internal EGR</td>
<td></td>
</tr>
</tbody>
</table>

**Input data**

**Engine performances:**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>EXP.</th>
<th>CALC.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Comp. Out. Press. [bar]</td>
<td>0.98</td>
<td>1.00</td>
</tr>
<tr>
<td>Turb. Inlet Temp [K]</td>
<td>565</td>
<td>564</td>
</tr>
<tr>
<td>Turb. Inlet Press. [bar]</td>
<td>0.97</td>
<td>1.06</td>
</tr>
<tr>
<td>IMEP [bar]</td>
<td>3.92</td>
<td>3.91</td>
</tr>
</tbody>
</table>
Test case

Model validation:

In cylinder pressure

Cumulative Burned Fuel Rate

In cylinder pressure during gas exchange

 Computational time:
 Only GT-Power 5 s/cycle
 Coupled run 40 s/cycle

Pentium IV 2 GHz
# Test case

Investigation on the possibility to use the Octane Number as a parameter for the engine control

**Engine operating conditions:**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>rpm</td>
<td>1500</td>
</tr>
<tr>
<td>Eng. Inlet Temp. [K]</td>
<td>310</td>
</tr>
<tr>
<td>Internal EGR</td>
<td></td>
</tr>
</tbody>
</table>

**Case 1:**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>Varied</td>
</tr>
<tr>
<td><strong>ON</strong></td>
<td>Varied according to the experiments</td>
</tr>
</tbody>
</table>

**Case 2:**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>3.72</td>
</tr>
<tr>
<td><strong>ON</strong></td>
<td>Varied</td>
</tr>
</tbody>
</table>
Test case

IMEP variation versus different LAMBDA values

Case 1:
Octane Number: varied
Lambda: varied

EGR composition influence on IGNITION CAD

Cylinder to cylinder variation
Test case

IGNITION CAD variation versus different OCTANE NUMBER values

Case 2:
Octane Number: varied
Lambda: 3.72

EGR composition influence on IGNITION CAD

Cylinder to cylinder variation
Test case

IN CYLINDER PRESSURES

IMEP versus LAMBDA

IGNITION CAD versus ON
Different heat transfer approach

**Ignition Code:**

**Stochastic Reactor Model (SRM)**

- Local Quantities: Temperature and mass fractions
  \[
  \Phi(t) = (\Phi_1, ..., \Phi_{S+1}) = (Y_1, ..., Y_S, T)
  \]

- Joint scalar Mass Density Function (MDF) \( F_\Phi(\Psi_1, ..., \Psi_{S+1}; t) \)

- Partially Stirred Plug Flow Reactor (PaSPFR)
  - Derived from PDF transport equation assuming statistical homogeneity

\[
\frac{\partial}{\partial t} F_\Phi(\Psi; t) + \frac{\partial}{\partial \Psi} \left( Q_i(\Psi) F_\Phi(\Psi; t) \right) = \frac{\partial}{\partial \Psi} \left( \frac{1}{1} C_\Phi (\Psi_i - \langle \Phi_i \rangle) F_\Phi(\Psi; t) \right)
\]

Source term: reaction, heat loss, \( dV \)

Mixing
Different heat transfer approach

Initial Temperature Distribution

Boundary Layer Treatment

- PDF Model: Stochastic Particles -
  - Bulk
  - Boundary layer

- Initial temperature distribution for the charge at IVC

- Differential cooling for the particles
Different heat transfer approach

Pressure & Emissions

In-cylinder pressure

CO, HC and NOx emissions

In-cylinder pressure

Emissions
Different heat transfer approach

Sensitivity w.r.t. number of particles

In-cylinder pressure: particle number sensitivity
- 11 particles
- 51 particles
- 101 particles

CO, HC and NOx emissions

In-cylinder pressure

Emissions

CO [g/kWh]  HC [g/kWh]  NOx [mg/kWh]

- 11 particles
- 51 particles
- 101 particles
Different heat transfer approach

ON variation

Engine operating conditions

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
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<tbody>
<tr>
<td>RPM</td>
<td>1500</td>
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<tr>
<td>ON</td>
<td>varied</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>3.72</td>
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<tr>
<td>Engine inlet temperature [K]</td>
<td>310</td>
</tr>
</tbody>
</table>

In-cylinder temperature sensitivity with respect to $ON$
Different heat transfer approach

ON variation analysis

Ignition crank angle degree

Combustion duration
Conclusions

• A computational tool for the calculation of ignition processes using a detailed kinetic mechanism was integrated into a commercial 1–D fluid–dynamics code

• Inhomogeneities in the local scalars are addressed by the PDF based stochastic reactor model thus enabling better agreement with the measured pressure and emissions as compared to a homogeneous full cycle engine model

• Computational time and results accuracy make the detailed kinetic model a useful tool for engine development
Future work

• Application of the kinetic model to every cylinder of the engine

• A Stochastic heat transfer model including the particle-wall interaction, effect preventing the assumption of an initial temperature profile

• Multi – zone model: application of the kinetic model to a certain number of zones in which the combustion chamber is divided. The zones differ as a consequence of the mass transfer, gas composition, heat transfer, etc...
Acknowledgement

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