Application of DARS 1D on in-cylinder combustion and aftertreatment

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Introduction

- **Aim**: To study the effect of $\lambda$ oscillation frequency in an SI engine on emission conversion in TWC.

- **Means**: 1D reactor network:

In-cylinder combustion → Piping → Three-way-catalyst (TWC)

CO conversion? NOx conversion? HC conversion?
All **engine** powertrain parts simulated with chemical kinetics

Models are **stochastic** ("SRM")

(detailed chemistry & short simulation times)

Species treated consistently from in-cylinder combustion to tail-pipe emission

Available engine models:

- SI
- DICI
- HCCI
- PPC
Methodology

1. Run SI SRM in-cylinder combustion model at $\phi = 0.98$, 1.00 and 1.02. Get outlet composition.

2. Make a step function of the outlet composition from fuel rich, fuel lean and stoichiometric composition. Impose the frequencies 1 Hz and 2 Hz, and use this as inlet to the pipe model.

3. Run the catalyst model with the outlet from the pipe model as input.
Methodology – in-cylinder combustion

SI SRM:
- Probability function based stochastic reactor model
- Relevant variables are spread over a number of virtual particles

Bjerkborn, S. et al., Predictive Flame Propagation Model for Stochastic Reactor Model Based Engine Simulations, ICDERS 2011, USA
Methodology – in-cylinder combustion

- Chemistry: Skeletal mechanism for PRF (iso-octane / n-heptane) blends [1] (238 species, 2197 reactions)
- Calculations at $\phi = 0.98$, 1.00 and 1.02.
- Get gas composition at EVO, use as input to pipe model

Results – in-cylinder combustion

Pressure trace for $\phi$ 0.98, 1.00 and 1.02.

Outlet mass fractions for $\phi$ 0.98, 1.00 and 1.02.

<table>
<thead>
<tr>
<th></th>
<th>$\phi = 0.98$</th>
<th>$\phi = 1.00$</th>
<th>$\phi = 1.02$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>5.35E-4</td>
<td>2.32E-3</td>
<td>6.90E-3</td>
</tr>
<tr>
<td>OH</td>
<td>4.48E-5</td>
<td>1.97E-5</td>
<td>6.87E-6</td>
</tr>
<tr>
<td>NO</td>
<td>3.91E-3</td>
<td>3.19E-3</td>
<td>2.49E-3</td>
</tr>
<tr>
<td>NO2</td>
<td>1.71E-5</td>
<td>1.10E-6</td>
<td>1.75E-7</td>
</tr>
</tbody>
</table>

118 s (9000 times real time) for one cycle on 8 CPU’s
The pipe is discretized into a number of cells. Each cell is a stochastic, constant volume PSR.

Chemistry calculated in each stochastic particle

Stochastic mixing and heat transfer to the walls
Methodology – exhaust piping

- Applying a step function, using the outlet composition from SI SRM as inlet composition
- Chemistry: Skeletal mechanism for PRF (iso-octane / n-heptane) blends [1] (238 species, 2197 reactions) - same as for in-cylinder combustion calculation
- Pipe length: 1 m
- Pipe diameter: 5 cm
- Cell length = 10 cm
- 20 particles per cell

### Results – exhaust piping

<table>
<thead>
<tr>
<th></th>
<th>Inlet</th>
<th>Exhaust</th>
<th>Conversion</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>6.90E-03</td>
<td>6.88E-03</td>
<td>2.4%</td>
</tr>
<tr>
<td>OH</td>
<td>4.48E-05</td>
<td>1.67E-08</td>
<td>99.96%</td>
</tr>
<tr>
<td>NO</td>
<td>3.91E-03</td>
<td>3.89E-03</td>
<td>0.51%</td>
</tr>
<tr>
<td>NO2</td>
<td>1.71E-05</td>
<td>4.75E-05</td>
<td>-177%</td>
</tr>
</tbody>
</table>

Maximum value of species mass fraction and conversion in pipe, 2Hz \( \phi \) oscillation.

- Emissions are not converted
- Radicals are converted
- Under fuel lean conditions NO is partially oxidized to NO\(_2\)

\( \phi \) oscillation (green line) and mass fraction CO, inlet and exhaust flow to/from the pipe, for \( \phi \) oscillation of 2 Hz.

1000 times slower than real time on 8 CPU’s
Transient 1D catalyst model

Three level solution:
- Reactor – conductive heat transfer
- Channel – flow and gas phase chemistry
- Washcoat – surface chemistry

The effect of $C_3H_6$ inhibition on NO reduction for lean exhaust gases in a Pt-Y-Alumina catalyst, 250 °C

Detailed and/or global reaction kinetics can be applied
Methodology – Three way catalyst

- Chemistry: A global TWC chemistry with oxygen storage [1] (9 gas phase species, 2 surface species, 9 global reactions + 6 surface reactions for oxygen storage)
- Unstable unburned hydrocarbons are lumped to the reference species $C_3H_6$
- Stable hydrocarbons are lumped to the reference species $C_3H_8$.
- Catalyst temperature = 850 K
- Exhaust gas temperature = 700 K
- Catalyst length = 10 cm
- Cell length = 0.5 cm

Results – Three way catalyst

- Significant difference between conversion at 1 and 2 Hz
- Overall conversion rate for CO is 54% higher at 2 Hz - oxygen storage

<table>
<thead>
<tr>
<th></th>
<th>1 Hz</th>
<th>2 Hz</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>44%</td>
<td>68%</td>
</tr>
<tr>
<td>NO</td>
<td>49%</td>
<td>49%</td>
</tr>
<tr>
<td>HC</td>
<td>85%</td>
<td>84%</td>
</tr>
</tbody>
</table>

Emission conversion in TWC

TWC inlet & outlet CO and NO mass fractions, at Φ oscillation of 1 and 2 Hz

240 times slower than real time on 1 CPU
Conclusions

- DARS 1D can be used to study the effect of $\lambda$ variations on TWC conversion performance
- DARS 1D can be used to in a consistent way study chemical effects in in-cylinder combustion, piping and aftertreatment systems
- Radicals are converted and NO is partially oxidized in the exhaust piping
- TWC performance is highly dependent on $\lambda$ oscillation frequency
- Total time for the project: ~1-2 man weeks
Thank you for your attention!

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