Using STAR-CCM+ for Catalyst Utilization Analysis

STAR Global Conference
Amsterdam – Netherlands
March 19-21 2012

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Background

- A number of years ago, Ford Motor Company (FMC) suffered a catalyst recall in North America.
- To avoid such issues happened again, a CFD-based method was developed to optimise catalyst gas flow distribution.
- The original methodology was based on under-floor exhaust systems but the current test procedure is applicable to hot-end designs with catalyst / filter, naturally aspirated / turbocharged, gasoline / diesel engines.
- The objectives of the test procedures are:
  - To have a robust and consistent approach to assess the performance of exhaust manifold/catalytic converter systems.
  - To optimise the design so that it can achieve the specified design targets.
  - To establish a systematic way to collect and to report data.
- The use of the CFD-based test procedure for exhaust Product Development (PD) is mandatory since 2003.
- The current test procedure is based on STAR-CD.
Design Variants

Close-coupled catalyst for an 1.6L I4 naturally aspirated gasoline application

Under floor catalyst for a 2.0L I4 turbocharged gasoline application

Close-coupled catalyst for an 3.5L V6 naturally aspirated gasoline application

After treatment system for an 2.2L I4 turbocharger diesel application
Benefits of Using CFD for Exhaust PD

- One key parameter to determine the exhaust after treatment system performance is the amount of precious materials (PGM) used in the catalyst.
- By combining the use of CFD in exhaust PD and other technology advancements in other areas, such as improved wash coat formulations and calibration techniques, a significant improvement in emissions performance and reduction in PGM cost and weight could be achieved.

Stage 4 TWC of 1.6L gasoline engine for B-car with cast exhaust manifold: 1.2L substrate, weighed 10.4 kg

Stage 5 TWC of 1.6L gasoline engine for B- and C-car with fabricated exhaust manifold: 1.0L substrate, weighed 5.3 kg
PGM Cost Reduction

PGM Cost of a Stage IV TWC after treatment system for a typical 1.6L gasoline engine from 1998 to 2006 Model Year

<table>
<thead>
<tr>
<th>Year</th>
<th>Total PGM Cost at CBP PGM rates</th>
<th>Total PGM Cost at April 06 PGM rates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1998 MY</td>
<td>$146.74</td>
<td>$113.76</td>
</tr>
<tr>
<td>2006 MY</td>
<td>$79.59</td>
<td>$69.78</td>
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</tbody>
</table>

Cost in $
Exhaust PGM & Total Costs between European OEMs

European OEM 1.6 Petrol St IV Catalyst Internals Estimated Costs - 2006 Model Year

<table>
<thead>
<tr>
<th>Model Year</th>
<th>European OEM 1.6 Petrol St IV Catalyst Internals Estimated Costs - 2006 Model Year</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PGM Cost (CBP rates)</td>
</tr>
<tr>
<td>2006</td>
<td>$36.73</td>
</tr>
<tr>
<td></td>
<td>$77.22</td>
</tr>
<tr>
<td>2007</td>
<td>$56.68</td>
</tr>
<tr>
<td></td>
<td>$39.51</td>
</tr>
<tr>
<td>2008</td>
<td>$24.01</td>
</tr>
<tr>
<td></td>
<td>$13.86</td>
</tr>
</tbody>
</table>

Courtesy of M. Brogan
Assumptions of the Current Approach

- Exhaust gas is represented by air.
- The gas flow in an exhaust system is of a transient nature but the analysis was simplified to a number of steady state analyses.
- Boundary conditions, such as mass flow rate, are adjusted according to the engine types, e.g. naturally aspirated or turbocharged.
- Chemical reactions are not included in the simulations.
- Standard k-epsilon turbulence model with high Y+ for near wall treatment.
- All wall boundaries are assumed to be adiabatic, e.g. No heat transfer.
- Substrate of the catalytic converter or filter, e.g. diesel particulate filter, is modelled as porous media.
- Pressure drop across an uncoated substrate under the specified operation condition is described by the following equation:
  \[ \Delta P/L = -(\alpha V + \beta) V \]
  \( \alpha \) and \( \beta \) are known as permeability coefficients
- Physical properties of the uncoated substrate are characterised by the open frontal area (OFA), hydraulic diameter (\( d_h \)) and material porosity.
- User subroutines are used to determine the pressure coefficients of the substrates.
Key Features of the Current Procedure

The procedure defines (or recommends) certain requirements for performing steady state CFD analysis, such as:

- Software requirements
- Modelling requirements
- Mesh requirements and quality
- Set-up requirements
- Modelling the substrate
- Boundary conditions
- Analysis requirements
- Post-processing
- Reporting format
Targets

• The key design targets (for analytical sign-off) are:
  – Flow Uniformity Index—A statistical measure of the gas flow distribution across the catalyst front face.
  – Velocity Index—Location of the high velocity flow and it should be kept away from the edge.

• Other design parameter:
  – Pressure drop values (system and across the catalyst/filter).

• Supporting information (reference only):
  – Velocity ratio, space velocity, annular velocity ratio etc.

Effects of flow mal-distribution on catalyst front-face

Effects of flow mal-distribution on mount durability
Objectives of the Upgrade

• To upgrade the analytical process from STAR-CD to STAR-CCM+ format.
• The new process shall maintain all STAR-CD key features, e.g.
  – User subroutine to determine the pressure coefficients
  – Post processing scripts
  – Ease to use
• As a minimum, the STAR-CCM+ version should replicate most (or ideally all) the things that STAR-CD version can do.
• Make use of the new modelling techniques, e.g. use Full Momentum instead of Darcy Law for porous material modelling.
• Using better approaches to determine the convergence.
• Ideally, the new process should have a minimum impact on the assessment procedure, e.g. use the same design target values.
• Reduce the turnaround time but maintain ‘quick and high quality’ analysis.
Current Status

Objectives which have been achieved so far:

– Maintain most of the Prostar/STAR-CD features, key exceptions are 1) use vertex to define value and 2) to calculate the Annular Velocity Ratio.
– Easy to use, one script for model set-ups etc and one script for analysis/post-processing.
– Scripts are used to define a large portion of the model set-ups.
– Applicable to designs with single (turbocharged) or multiple runners (naturally aspirated).
– Applicable to single and multiple catalyst/filter after treatment systems.
– Volume meshing (including porous material region) is fully automated.
– Using field functions to define the pressure coefficients, catalyst (ready), filter (in progress).
– Unique method to determine the ‘true’ centre of the catalyst cross-section.
– Three ways to define the Stopping Criteria.
– Using field functions to perform the post processing.
– Scripts to create all the data for reporting.
– Perform volume meshing/analysis/post-processing in batch mode.
– The current design target values are applicable.
Work Flow

**Preparation: Parts need user's input**

- Import the surface model and label the regions with appropriate names
- Define the options and values for surface re-meshing and volume meshing
- Define the options and values for boundary conditions and initialization

**GUI controlled with few user inputs required**

- Run the GUI to define the substrate properties and choose the default model set-ups option
- Perform the analysis
- Post-processing

- Use the results to prepare a summary report for review
- Additional model set-ups?
  - NO
  - YES
    - Modify the model set-ups via CCM+’s (optional)
GUI Panel

- **Version number**
- **Mesh status**
- **Number of runners and substrates**
- **Options to define the substrate properties (unique ID). One has to repeat this step for cases with multiple substrates**
- **Option to use default model set-ups and number of iterations**
- **Option to set up pre-swirl at the inlet region**
- **Perform analysis with and without post-processing**

**N.B.** The GUI panel should be called within the CCM+
Geometry of the Test Case

The geometry is based on a close-coupled diesel oxidation catalyst of an after treatment system for a 2.0L turbo-diesel engine.
Define the Locate Coordinate System

Local coordinate system defined by the user in CCM+ will be transferred to the true cross-section centre by using the GUI.
# STAR-CD vs. STAR-CCM+

![Images of flow distribution](image1.png) ![Images of flow distribution](image2.png) ![Images of flow distribution](image3.png) ![Images of flow distribution](image4.png)

## Comparison Table

<table>
<thead>
<tr>
<th>Case ID</th>
<th>Solver</th>
<th>Mesh (main)</th>
<th>Mesh (substrate)</th>
<th>Diff. scheme</th>
<th>Turbulence model</th>
<th>Near wall treatment</th>
<th>Uniformity Index</th>
<th>Velocity Index</th>
<th>Averaged flow velocity (m/s)</th>
<th>System pressure drop (kPa)</th>
<th>Pressure drop across the substrate (kPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ID 1.01</td>
<td>STAR-CD</td>
<td>Hexa</td>
<td>Hexa</td>
<td>First</td>
<td>Standard k-ε</td>
<td>High Y+</td>
<td>0.91</td>
<td>0.99</td>
<td>15.57</td>
<td>11.47</td>
<td>2.32</td>
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<tr>
<td>ID 1.06</td>
<td>STAR-CCM+</td>
<td>Poly</td>
<td>Poly</td>
<td>First</td>
<td>Standard k-ε</td>
<td>High Y+</td>
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<td>0.95</td>
<td>15.54</td>
<td>11.15</td>
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<td>ID 1.21</td>
<td>STAR-CCM+</td>
<td>Poly</td>
<td>Poly</td>
<td>First</td>
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<td>0.95</td>
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<td>ID 1.11</td>
<td>STAR-CCM+</td>
<td>Poly</td>
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<td>Second</td>
<td>Standard k-ε</td>
<td>High Y+</td>
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<td>0.95</td>
<td>15.72</td>
<td>9.04</td>
<td>2.37</td>
</tr>
</tbody>
</table>
Conclusions

• In the past several years, Ford used a CFD-based test procedure for catalyst utilization and similar analysis.
• The use of the such test procedure for design sign-off has been proved very successful.
• The CFD procedure for catalyst utilization has been upgraded to STAR-CCM+ format.
• The new procedure has maintained most of the key features as found in the current procedure, such as using physical data to define the pressure coefficients, scripts for post-processing etc.
Thank you for your attention.
Any questions?