Soot Mass Limit Prediction via Coupled Thermo-Mechanical Stress Analysis

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Background and motivation

- DPF overheating failure modes
  - Local melting
  - Cracks

- Parameters affecting DPF failure
  - Geometry
    - Diameter, length, cell density, wall thickness
    - Segmentation
  - Material properties
    - Substrate wall material, porosity
    - Cement
  - Operating parameters
    - Exhaust flow rate
    - Oxygen content
    - Temperature
    - Soot loading, distribution
    - ...

- Experimental methods are ‘inherently’ destructive and cost-intensive

Mizutani et al, SAE paper 2006-01-1527
Contents

- DPF regeneration modeling
- Thermomechanical stress prediction
- Demonstration case
- Parametric analysis
- Results - conclusions
Overview of DPF model equations

**Filter scale: 3-d solid energy balance**

\[
\rho_s \cdot C_{p,s} \frac{\partial T_s}{\partial t} = k_{s,x} \frac{\partial^2 T_s}{\partial x^2} + k_{s,y} \frac{\partial^2 T_s}{\partial y^2} + k_{s,z} \frac{\partial^2 T_s}{\partial z^2} + S
\]

\[
S = H_{\text{conv}} + H_{\text{wall}} + H_{\text{react}} + H_{\text{rad}}
\]

**Channel scale: gas balances**

**Mass/momentum/energy/species**

\[
\frac{\partial}{\partial z} \left( d_i^2 \rho_i v_i \right) = (-1)^j 4d_i \rho_w v_w
\]

\[
\frac{\partial}{\partial z} \left( \rho_i v_i^2 \right) = -\alpha_i \nu_i I d_i^2
\]

\[
C_{p,g} \rho_i v_i \left| \frac{\partial T_i}{\partial z} \right| = h_i \frac{4}{d_i} (T_s - T_i)
\]

\[
C_{p,g} \rho_2 v_2 \left| \frac{\partial T_2}{\partial z} \right| = (h_2 + C_{p,g} \rho_w v_w) \frac{4}{d} (T_s - T_2)
\]

\[
\frac{\partial}{\partial z} \left( v_i y_{1,j} \right) = -\frac{1}{d_{f_{-w}}} v_w y_{1,j} + \frac{1}{d_{f_{-w}}} k_{1,j} (y_{1s,j} - y_{1,j})
\]

\[
\frac{\partial}{\partial z} \left( v_2 y_{2,j} \right) = -\frac{1}{d_{f_{+w}}} v_w y_{2s,j} + \frac{1}{d_{f_{+w}}} k_{2,j} (y_{2s,j} - y_{2,j})
\]

**Wall/soot scale balances**

**Momentum/soot/ species**

\[
\frac{dp}{dx} = \mu v(x)
\]

\[
\frac{d\dot{m}_p}{dt} = -\dot{m}_p \sum R'_k + s_p \rho_w v_w \mu_p
\]

\[
v_w \frac{\partial y_{1,j}}{\partial x} - D_j \frac{\partial}{\partial x} \left( f_s \frac{\partial y_{1,j}}{\partial x} \right) = f_s \sum_{k} c_{i,k} R_k
\]

Soot oxidation kinetics (CLEERS, 2010)

Experimental procedures for efficient after-treatment model calibration

Methodology: Use of real diesel soot collected in real filter; oxidation with synthetic gas; model calibration; engine test validation.

Results: Two mechanisms of soot oxidation with O2; calibration of C+NO2 reaction.
3-Dimensional Modeling of the Regeneration in SiC Particulate Filters

Aristotle University Thessaloniki, Greece
C.-D. Vogt, E. Ohara
NGK Europe GmbH, Germany
Y. Watanabe, T. Mizutani
NGK Insulators Ltd., Japan

Model validation – centerline channel
Initial soot loading: 8 g/l

Test protocol

3 different initial soot loadings: 4, 6, 8 grams/liter

Correlation of maximum temperature at each position

Dots: Measurement, Lines: Model

Compared maximum temperature (°C)

Measured maximum temperature (°C)

3 different initial loadings
DPF regeneration model applications

**HD application**
Multi-dimensional regeneration modeling validation (CaPoC 5, 2006)

**LD application**
DPF protection from overheating by heating measures (SAE 2007)
Contents

- DPF regeneration modeling
- **Thermomechanical stress prediction**
- Demonstration case
- Parametric analysis
- Results - conclusions
Stress analysis
Definitions and model assumptions

- **Thermal expansion coefficient:**
  \[ \alpha = \frac{1}{L} \frac{dL}{dT} \]

- **Young's modulus:** measure of material stiffness, ratio of the tensile stress over tensile strain:
  \[ E = \frac{\sigma}{\varepsilon} \]

- **Shear modulus** is the ratio of shear stress to the shear strain

- **Poisson's ratio:** transverse to longitudinal strains

<table>
<thead>
<tr>
<th>Orthotropic material equations for channel region</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young's modulus</td>
</tr>
<tr>
<td>[ E_R = E_{\theta} = E_s \frac{w_s}{w_s + D} ]</td>
</tr>
<tr>
<td>[ E_Z = E_s \frac{2(w_s + D)w_s - D^2}{(w_s + D)^2} ]</td>
</tr>
<tr>
<td>Shear modulus</td>
</tr>
<tr>
<td>[ G_{\theta Z} = E_{R\theta} = G_s \frac{w_s}{D} ]</td>
</tr>
<tr>
<td>[ G_{RZ} = G_s \frac{w_s^3}{2(w_s + D)^3} ]</td>
</tr>
<tr>
<td>Poisson's ratio</td>
</tr>
<tr>
<td>[ \nu_{R\theta} = \nu_{Z\theta} = \nu_s ]</td>
</tr>
<tr>
<td>[ \nu_{R\theta} = \nu_{\theta R} = \nu_s \frac{w_s}{w_s + D} ]</td>
</tr>
<tr>
<td>[ \nu_{Rz} = \nu_{\theta Z} = \nu_s \frac{1}{2 - \frac{w_s}{w_s + D}} ]</td>
</tr>
</tbody>
</table>

Kim J. S., SAE paper 2004-01-1134
SAE 2012-01-1252: Failure stress and apparent elastic modulus of Diesel Particulate Filter Ceramics (Wereszczak et al., ORNL)

<table>
<thead>
<tr>
<th>CORDIERITE DPF</th>
<th>Elastic Modulus [GPa]</th>
<th>Tensile Failure Stress [MPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quasi-static/Mechanical Equibiaxial Flexure (Axial direction)</td>
<td>0.5-1.5</td>
<td>2 (Interior structure) &gt;4 (50% end fill radial)</td>
</tr>
<tr>
<td>Quasi-static/Mechanical Sectored Flexure (Radial direction)</td>
<td>1-3 (Interior structure) 4-24 exterior skin</td>
<td>5-13 (Exterior skin axial)</td>
</tr>
<tr>
<td>Quasi-static/Mechanical O-Ring Flexure (Tangential direction)</td>
<td>1.1-2.1</td>
<td>2-4</td>
</tr>
</tbody>
</table>
Stress analysis
‘Conventional’ workflow

FEA grid generator
• Custom, user-dependent scripting

Temperature field data

Data processor

Stress analysis solver
• Abaqus
• Nastran
• ANSYS
• ...
  • FEA knowhow

Visualization tool
• Tecplot
• Paraview
• ...
  • Additional cost
  • User experience

Measured data
• Expensive
• Destructive

Simulation data
• Time consuming
Integrated simulation approach
‘CAE-intensive’

- Engine-out data w/o aftertreatment
- 3d DPF model
- Data processor
- Stress analysis solver
- Customized visualization tool
Integrated simulation approach ‘CAE-intensive’

Engine-out data w/o aftertreatment

3d DPF model

Data processor

Stress analysis solver

DYNAMIS

Customized visualization tool

<table>
<thead>
<tr>
<th></th>
<th>CPUs</th>
<th>Simulation time [s]</th>
<th>Grid</th>
<th>CPU time</th>
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</thead>
<tbody>
<tr>
<td>axitraps</td>
<td>4</td>
<td>600</td>
<td>4 chan/node</td>
<td>≈ 1 hr</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>130,000 nodes</td>
<td></td>
</tr>
<tr>
<td>Dynamis</td>
<td>4</td>
<td>300</td>
<td>130,000 nodes</td>
<td>≈ 1 hr</td>
</tr>
</tbody>
</table>
Sensitivity of simulation results to mesh discretization

**Temperature gradient [°C]**

- **Maximum wall temperature [°C]**
  - 1D: 47000
  - 2D: 130000
  - 3D: 21000
  - 4D: 418500

**Maximum stress [GPa]**

- Finer mesh, computationally expensive
  - 3D: 3.1
  - 4D: 3.6

Not critical for peak temperature prediction accuracy

Necessary for stress prediction accuracy
Contents

- DPF regeneration modeling
- Thermomechanical stress prediction
- Demonstration case
- Parametric analysis
- Results - conclusions
### Geometrical data

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>DOC</td>
<td>V = 3.1 l</td>
<td>L=76 mm</td>
</tr>
<tr>
<td></td>
<td>D=228 mm</td>
<td>400/6 cpsi/mil</td>
</tr>
<tr>
<td>DPF</td>
<td>V = 8.3 l</td>
<td>L=203 mm</td>
</tr>
<tr>
<td></td>
<td>D=228 mm</td>
<td>200/15 cpsi/mil</td>
</tr>
<tr>
<td></td>
<td>d_{Skin} =1.5 mm</td>
<td>No. segments=9</td>
</tr>
</tbody>
</table>

### DPF Material properties

| Substrate (SiC) | Porous wall density [kg/m$^3$] | 1900 |
|                | Poisson ratio [-]              | 0.15 |
|                | Thermal expansion coefficient [1/K] | 4 10$^{-6}$ |
|                | Young modulus [GPa]            | 10   |
| Cement         | Density [kg/m$^3$]             | 1260 |
|                | Poisson ratio [-]              | 0.2  |
|                | Thermal expansion coefficient [1/K] | 2.7 10$^{-6}$ |
|                | Young modulus [GPa]            | 1.5  |
| Skin           | Same as cement                 |      |
| Insulation     | Fibermat                       |      |
| Canning        | Stainless steel                |      |
Due to the relatively low flow rate, the temperature increases excessively and the regeneration rates are fast. Highest temperatures near filter exit.
Soot loading and temperature distribution
Initial soot loading: 10.5 g/l
Flow distribution and gas outlet temperature
Initial soot loading: 10.5 g/l
Axial stress analysis results
Initial soot loading: 10.5 g/l
Radial stress analysis results
Initial soot loading: 10.5 g/l
The stress analysis model results are in line with experimental DPF failure observations.
Determination of soot mass limit
Maximum axial stress vs time

Soot mass limit for ring-off cracks: 9.5 g/l
Parametric analysis
Assumptions and parameters varied

Parameters kept constant as reference case
- All inlet gas conditions
- DOC
- DPF external dimensions
- DPF cell structure
- Initial soot loading

Parameters varied in the parametric analysis
- Number of segments
- Wall porosity: 42% to 70%
- Cement thermal expansion coefficient: 25% to 400% of baseline value

The soot mass limit is evaluated for axial stresses only.
Variation of DPF segments: Temperature fields at the occurrence of peak temperature.

Obvious influence of segmentation due to cement heat capacity and insulating effect.
Axial stresses for different segmentations. 9.5g/l, time of peak stress occurrence

Highest stresses calculated close to the segment boundaries (region of high temperature gradients)
Calculated soot mass limit as function of number of segments

Significant impact of segmentation on soot mass limit.
Mechanical failure not directly correlated to max. wall temperature
Segmentation optimization is subject to additional factors: cost, pressure drop etc.
### Wall porosity effect
What is affected by the variation of wall porosity

<table>
<thead>
<tr>
<th>Property</th>
<th>Equation</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wall density</td>
<td>$d(\varepsilon) = d_0 (1 - \varepsilon)$</td>
<td></td>
</tr>
<tr>
<td>Wall conductivity [W/mK]</td>
<td>$k(\varepsilon) = k_0 (1 - \varepsilon)$</td>
<td></td>
</tr>
<tr>
<td>Young modulus [GPa]:</td>
<td>$E(\varepsilon) = E_0 \frac{(1-\varepsilon)^2 R}{\varepsilon + (1-\varepsilon) R}$</td>
<td>$E_0$: pore free Young modulus</td>
</tr>
<tr>
<td>Fracture strength [MPa]</td>
<td>$\sigma(\varepsilon) = \sigma_0 \frac{(1 - \varepsilon)^2 R}{\varepsilon + (1 - \varepsilon) R}$</td>
<td>$\sigma_0$: pore free Fracture strength</td>
</tr>
</tbody>
</table>

\( \varepsilon \): porosity
\( E_0 \): pore free Young modulus
\( \sigma_0 \): pore free Fracture strength
\( R \): particle size ratio

Predicted temperature fields at the occurrence of max stress

The lower thermal mass of the more porous substrates results in higher temperatures.
Axial stress for different wall porosities (9.5 g/l, snapshots at peak stress occurrence)
Soot mass limit vs. wall porosity

Significant impact of wall porosity on soot mass limit. Mechanical failure not directly correlated to max. wall temperature. Porosity optimization is subject to additional factors: filtration, pressure drop, coating etc.
Cement material properties are important on the thermomechanical stress behavior of the DPF. Material optimization is towards to the increase the cement stress absorption:

1. Young’s modulus
2. Thermal expansion coefficient

<table>
<thead>
<tr>
<th>Cement thermal expansion coefficient [1/K]</th>
<th>400%</th>
<th>200%</th>
<th>100%</th>
<th>50%</th>
<th>25%</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.08 $10^{-05}$</td>
<td>5.40 $10^{-06}$</td>
<td>2.70 $10^{-06}$</td>
<td>1.35 $10^{-06}$</td>
<td>6.75 $10^{-07}$</td>
</tr>
</tbody>
</table>

Mizutani et al, SAE paper 2006-01-1527
Axial stresses for different cement TCE. 9.5 g/l, peak stress occurrence

High cement CTE increase the stresses in the DPF substrate
The soot mass limit can be substantially affected by the properties of the cement layer.
Conclusions

- DPF stress analysis is facilitated by integrated CAE approaches with seamless model integration and short calculation times.
- The estimation of equivalent mechanical material properties and fracture limits is challenging for real DPF structures.
- The simulations provide reasonable agreement with experimental observations for peak stress location and overall trends.
- The effect of segmentation, wall porosity and cement properties were analyzed with respect to both thermal and mechanical stress effects during regeneration.
- Assisted by advances in the better understanding of material properties, simulation concepts could play a bigger role in DPF durability analysis and system optimization.
Acknowledgement

GSRT/Greek Ministry of Education (project 26SMEs2009: ‘Emission control system durability assessment’) for financial support.
Thank you for your attention!

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