Soot Mass Limit Prediction via Coupled Thermo-Mechanical Stress Analysis

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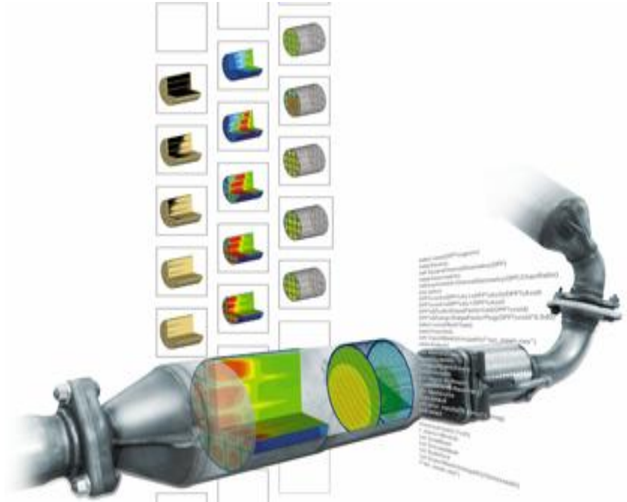
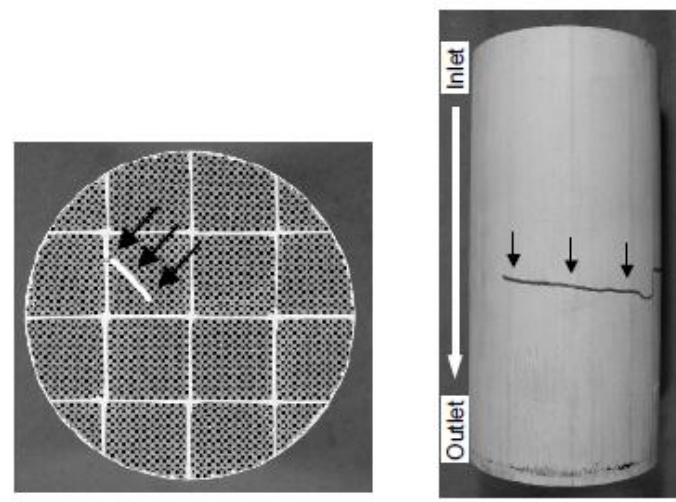


Background and motivation

- 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

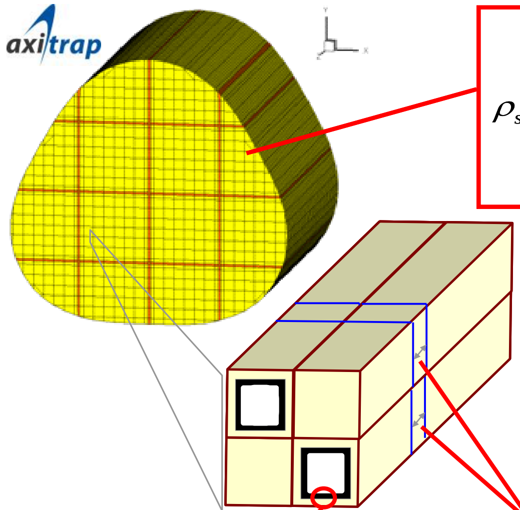


Mizutani et al, SAE paper 2006-01-1527

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

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

$$S = H_{conv}+H_{wall}+H_{react}+H_{rad}$$

Channel scale: gas balances
Mass/momentum/energy/species

$$\frac{\partial}{\partial z}\left(d_i^{\,2}\rho_i v_i\right) = (-1)^i\, 4d\rho_w v_w$$

$$\frac{\partial p_i}{\partial z}+\frac{\partial}{\partial z}\left(\rho_i v_i^2\right) = -\alpha_1\mu v_i / d_i^{\,2}$$

$$C_{p,g}\rho_1 v_1\big|_z \frac{\partial T_1}{\partial z} = h_1\frac{4}{d_1}(T_s-T_1)$$

$$C_{p,g}\rho_2 v_2\big|_z \frac{\partial T_2}{\partial z} = (h_2 + C_{p,g}\rho_w v_w)\frac{4}{d}(T_s-T_2)$$

$$\frac{\partial}{\partial z}\left(v_1 y_{1,j}\right) = -\frac{1}{df_{-w}^{\;2}} v_w y_{1,j} + \frac{1}{df_{-w}} k_{1,j}\left(y_{1s,j}-y_{1,j}\right)$$

$$\frac{\partial}{\partial z}\left(v_2 y_{2,j}\right) = \frac{1}{df_{w_s}^{\;2}} v_w y_{2s,j} + \frac{1}{df_{w_s}} k_{2,j}\left(y_{2s,j}-y_{2,j}\right)$$

Wall/soot scale balances
Momentum/soot/ species

$$\frac{dp}{dx}=\frac{\mu v(x)}{k_p}$$

$$\frac{d\hat m_p}{dt} = -\hat m_p\sum R'_k + s_F\rho_w v_w \mu_p$$

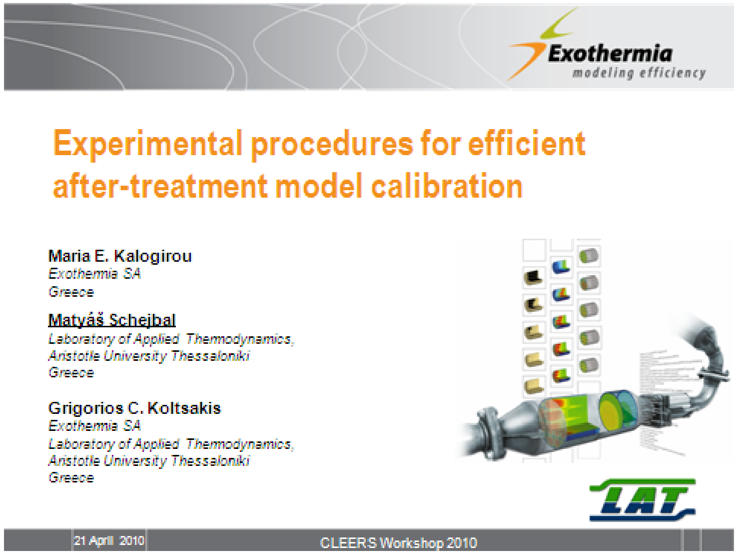
$$v_w\frac{\partial y_j}{\partial x} - D_j\frac{\partial}{\partial x}\left(f_x\frac{\partial y_j}{\partial x}\right) = \frac{f_x}{c_m}\sum_k c_{j,k}R_k$$

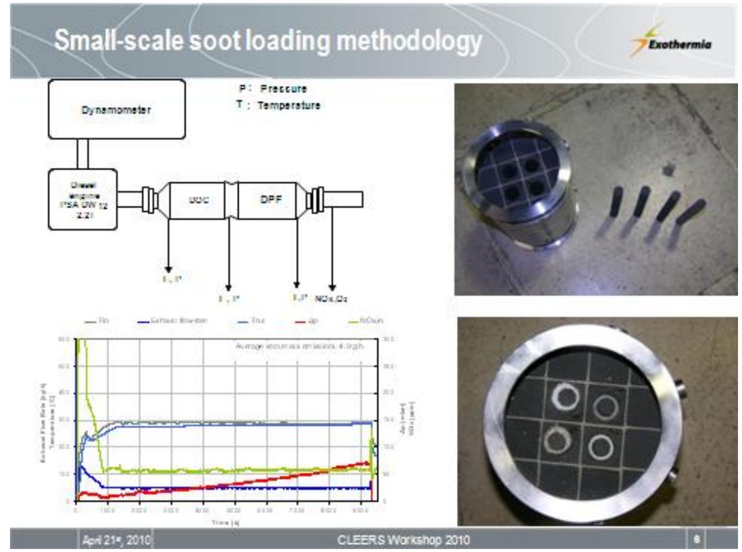
axisuite

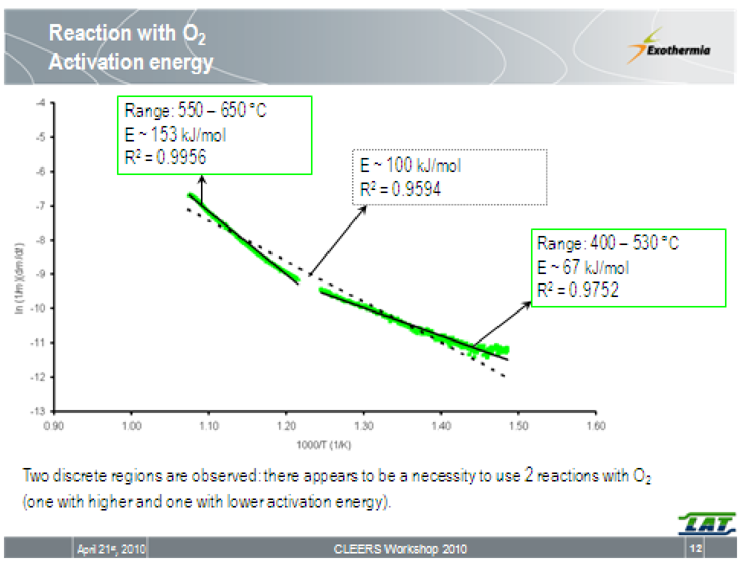
software module	functionality / reactor type	3-way catalyst	diesel oxidation catalyst	lean NO_x trap	selective catalytic reduction	diesel particulate filter
axicat	flow-through	✓	✓	✓	✓	n/a
axitrap	wall-flow	n/a	✓	✓	✓	✓
axifoam	deep-bed	n/a	✓	✓	✓	✓
axiheat	exhaust pipe	single-wall	double-wall	insulating material	flanges	reacting flow

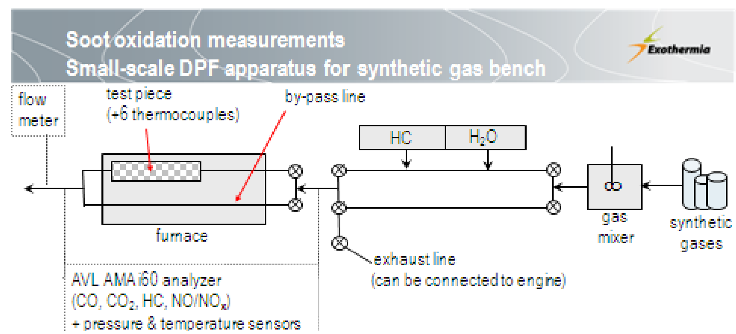
Koltsakis & Stamatelos A. M., *Ind. Eng. Chem. Res*., 1997 Vol. 36 p. 4155-4165.
Koltsakis et al, SAE 2003-01-1881, Haralampous et al., SAE 2004-01-0696, Koltsakis et al, SAE 2005-01-1881

Soot oxidation kinetics (CLEERS, 2010)









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.

3d thermal field prediction during regeneration (SAE 2005)

Exothermia

2005-01-0953

3-Dimensional Modeling of the Regeneration in SiC Particulate Filters

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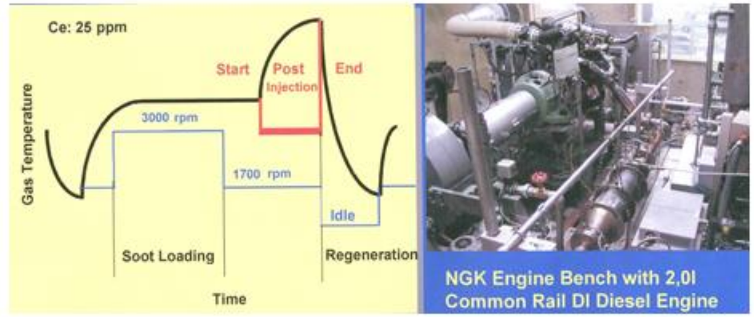
Aristotle University Thessaloniki, Greece
C.-D. Vogt, E. Ohara
NGK Europe GmbH, Germany
Y. Watanabe, T. Mizutani
NGK Insulators Ltd, Japan

SAE 2005 WORLD CONGRESS

Test protocol



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

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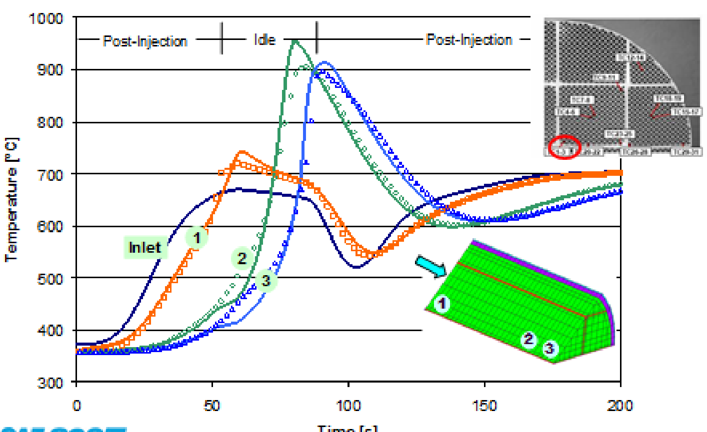
Model validation – centerline channel
Initial soot loading: 8 g/l



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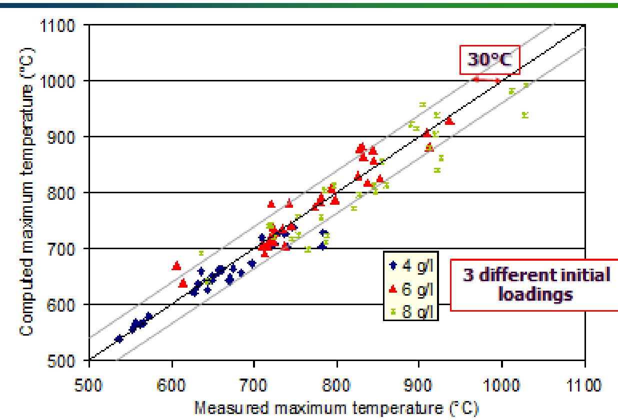
Dots: Measurement, Lines: Model

Measurement vs model
Correlation of maximum temperature at each position



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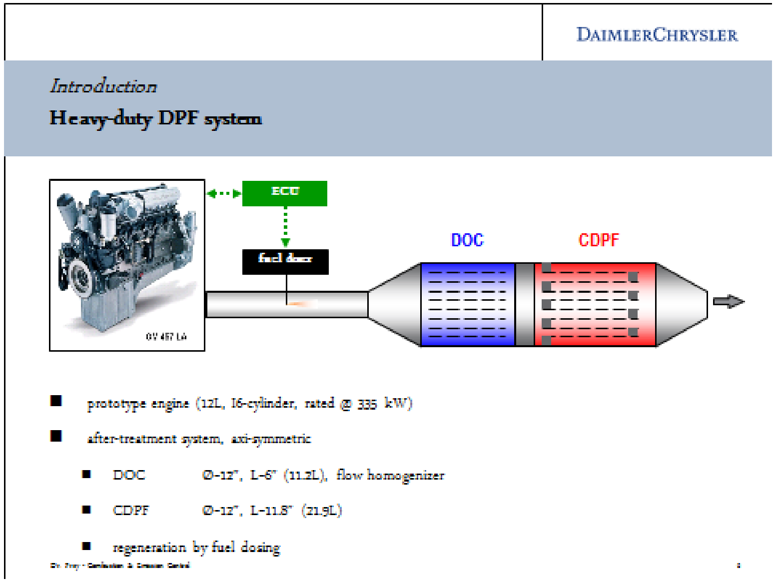
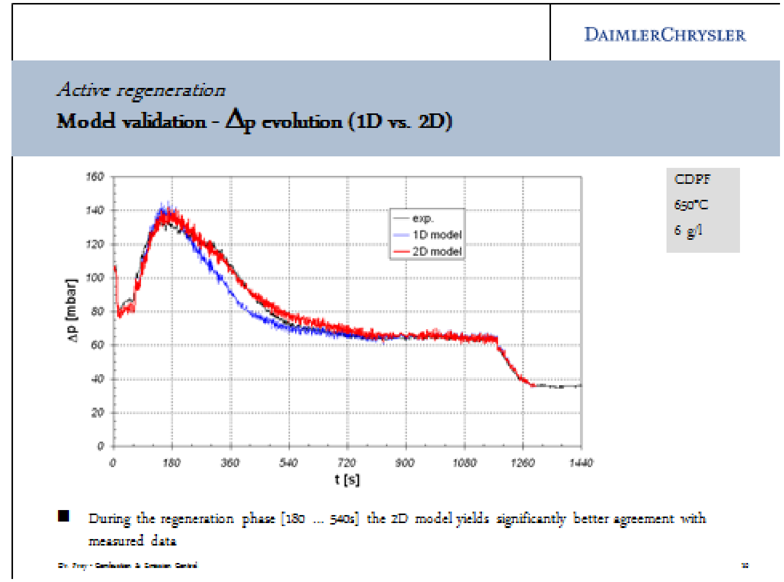
DPF regeneration model applications

Exothermia

HD application

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

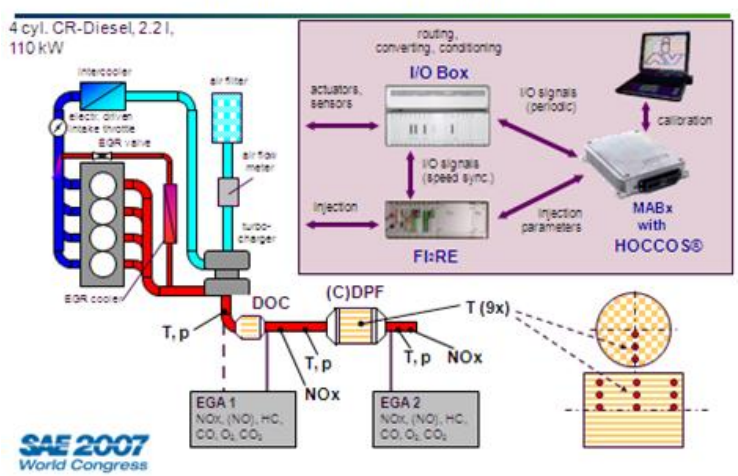




LD application

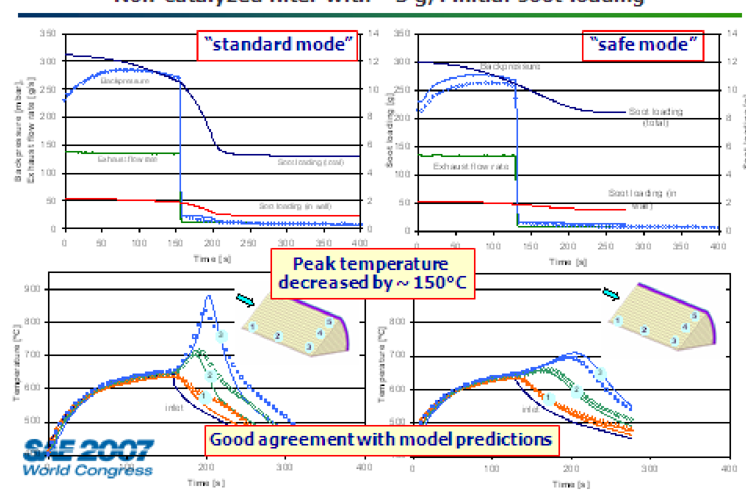
DPF protection from overheating by heating measures (SAE 2007)

Schematic test bench set-up at IAV



Experimental vs simulation results

Non-catalyzed filter with ~5 g/l initial soot loading



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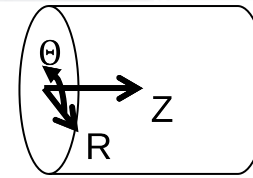
Stress analysis
Definitions and model assumptions



- **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

Orthotropic material equations for channel region	
Young's modulus	$E_R = E_\Theta = E_s \frac{w_s}{w_s + D}$
	$E_Z = E_s \frac{2(w_s + D)w_s - D^2}{(w_s + D)^2}$
Shear modulus	$G_{\Theta Z} = E_{R\Theta} = G_s \frac{w_s}{D}$
	$G_{RZ} = G_s \frac{{w_s}^3}{2\,(w_s + D)^3}$
Poisson's ratio	$v_{R\Theta} = v_{Z\Theta} = v_s$
	$v_{R\Theta} = v_{\Theta R} = v_s \frac{w_s}{w_s + D}$
	$v_{Rz} = v_{\Theta z} = v_s \frac{1}{2 - \frac{w_s}{w_s + D}}$

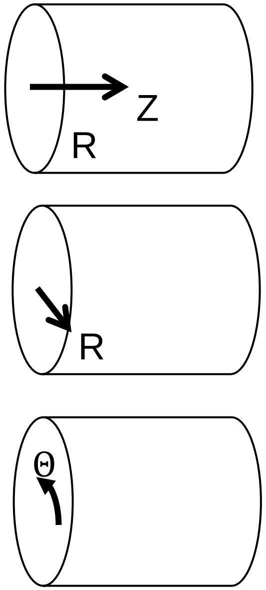
w_s : wall thickness
D: channel diameter

Kim J. S., SAE paper 2004-01-1134

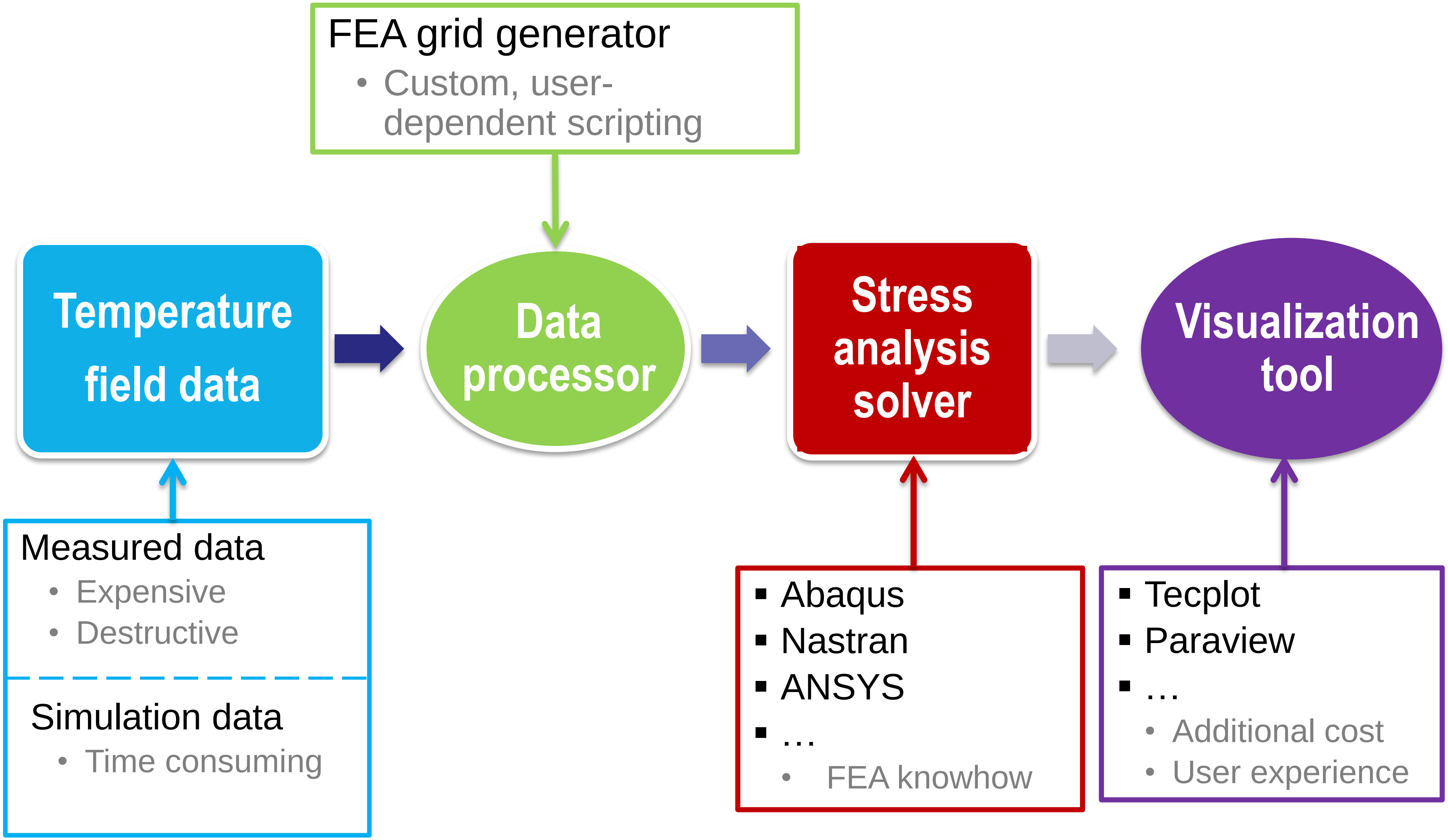
Material properties

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

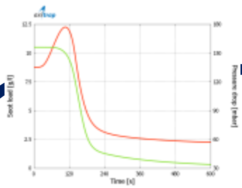
CORDIERITE DPF	Elastic Modulus [GPa]	Tensile Failure Stress [MPa]
Quasi-static/Mechanical Equibiaxial Flexure (Axial direction)	**0.5-1.5**	**2** (Interior structure) **>4** (50% end fill radial)
Quasi-static/Mechanical Sectored Flexure (Radial direction)	**1-3** (Interior structure) **4-24** exterior skin	**5-13** (Exterior skin axial)
Quasi-static/Mechanical O-Ring Flexure (Tangential direction)	**1.1-2.1**	**2-4**



Stress analysis
‘Conventional’ workflow



Integrated simulation approach 'CAE-intensive'



Engine-out data w/o aftertreatment

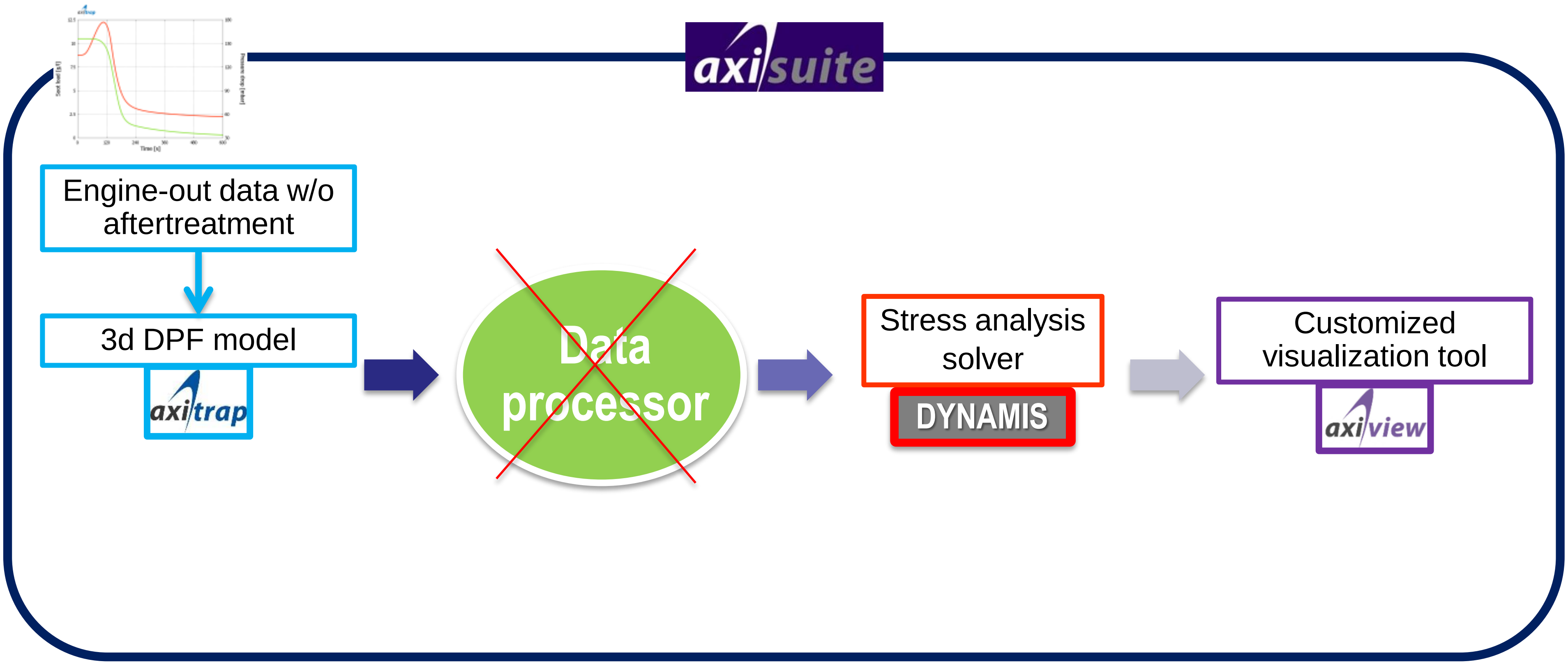
3d DPF model

Data processor

Stress analysis solver

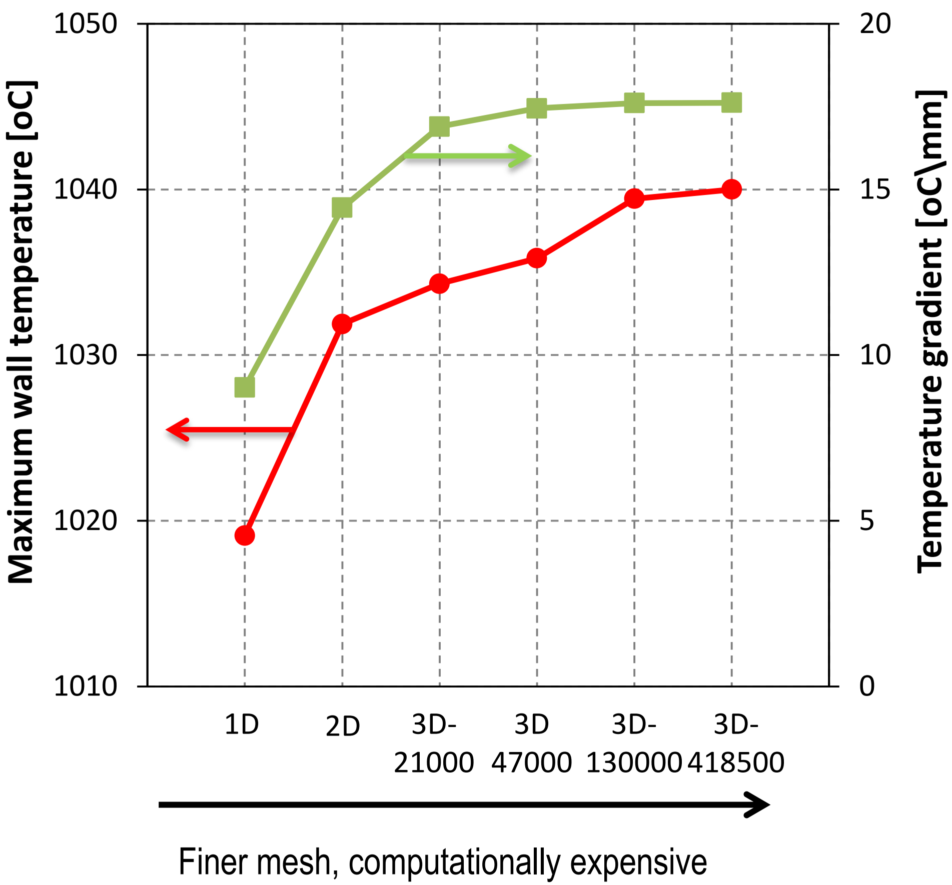
Customized visualization tool

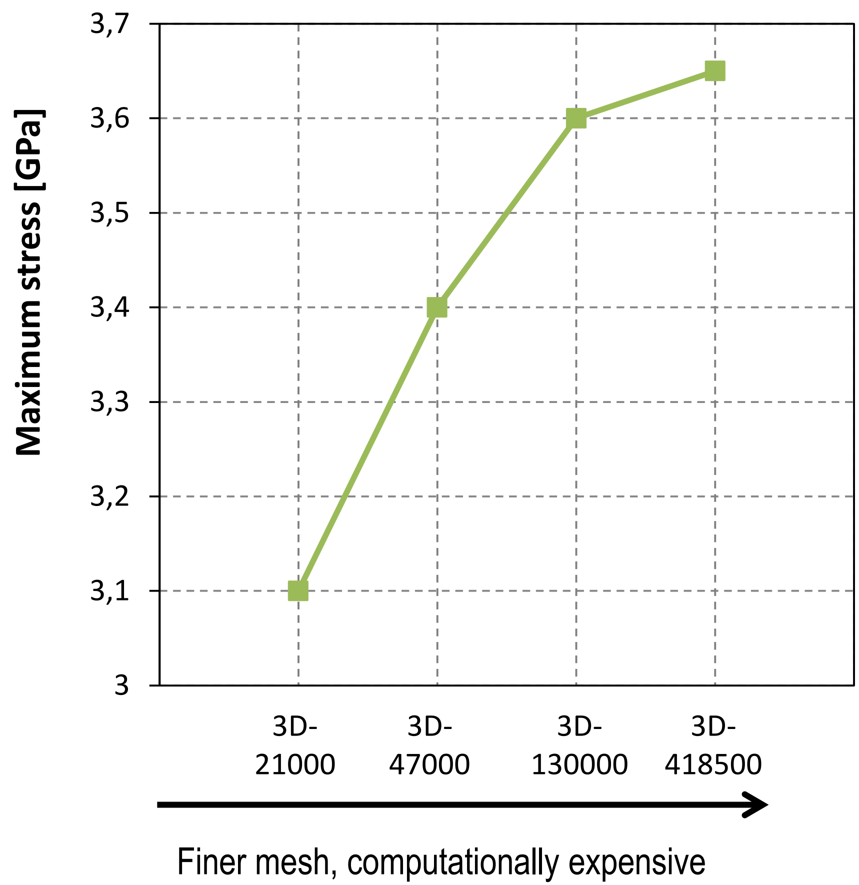
Integrated simulation approach ‘CAE-intensive’



	CPUs	Simulation time [s]	Grid	CPU time
axitrap	4	600	4 chan/node 130,000 nodes	≈ 1 hr
Dynamis	4	300	130,000 nodes	≈ 1 hr

Sensitivity of simulation results to mesh discretization





Not critical for
peak temperature prediction accuracy

Necessary for
stress prediction accuracy

Contents

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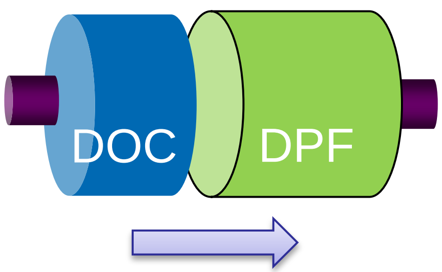
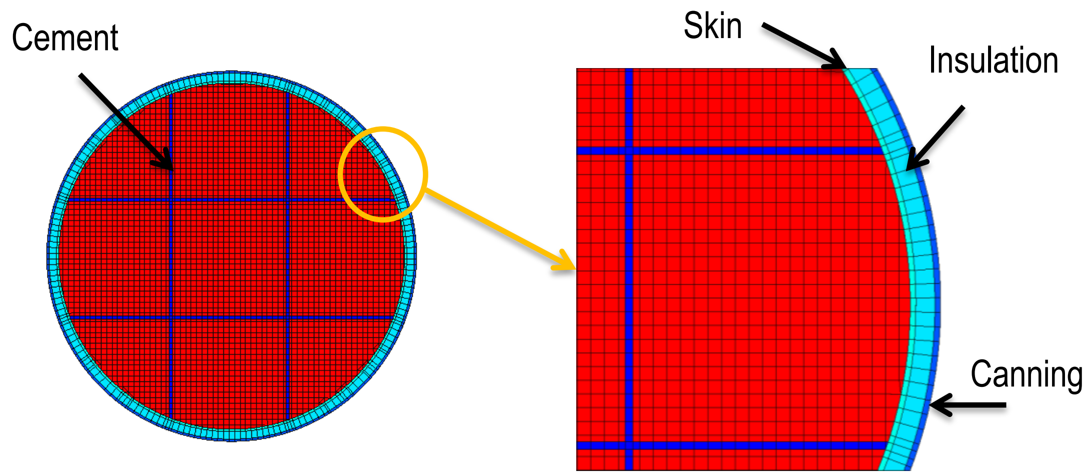
- **Demonstration case**
- Parametric analysis
- Results - conclusions

Basic geometry and material data

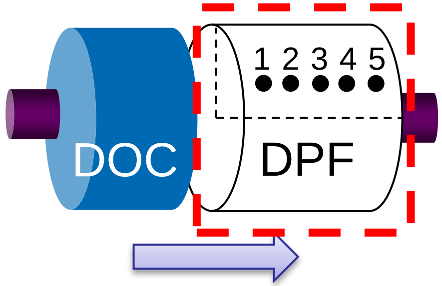


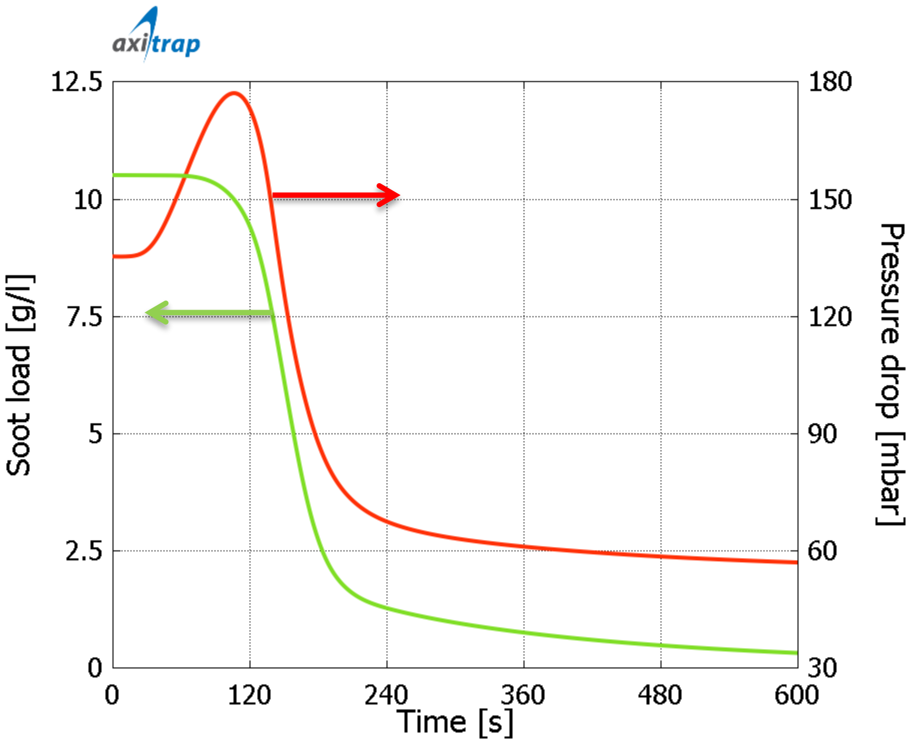


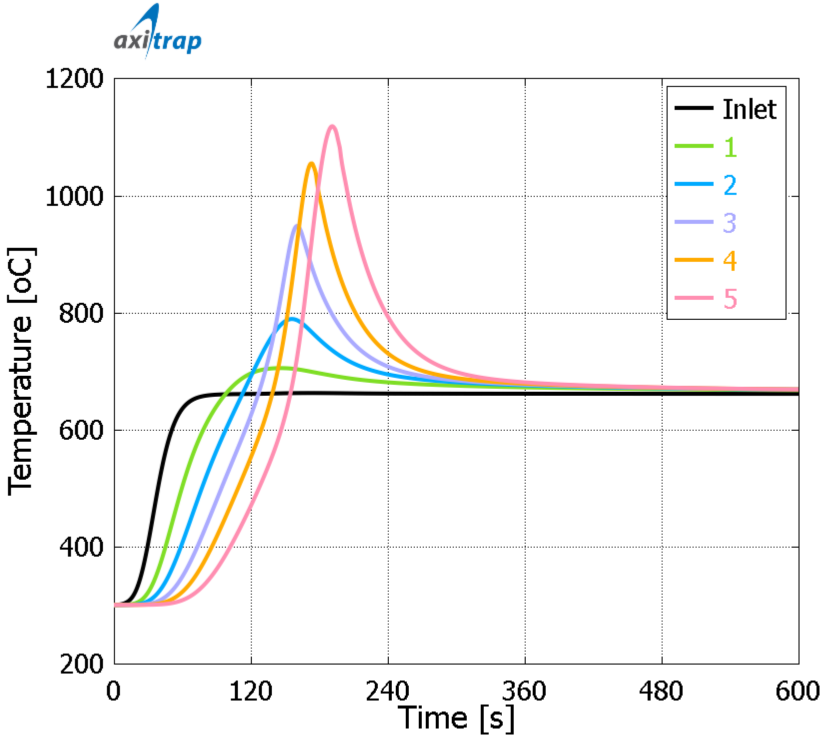
Geometrical data	
DOC	V = 3.1 l L=76 mm D=228 mm 400/6 cpsi/mil
DPF	V = 8.3 l L=203 mm D=228 mm 200/15 cpsi/mil d_{Skin} =1.5 mm No. segments=9

DPF Material properties		
Substrate (SiC)	Porous wall density [kg/m^3] Poisson ratio [-] Thermal expansion coefficient [1/K] Young modulus [GPa]	1900 0.15 $4\ 10^{-6}$ 10
Cement	Density [kg/m^3] Poisson ratio [-] Thermal expansion coefficient [1/K] Young modulus [GPa]	1260 0.2 $2.7\ 10^{-6}$ 1.5
Skin	Same as cement	
Insulation	Fibermat	
Canning	Stainless steel	

DPF simulation: reference case
Initial soot loading: 10.5 g/l

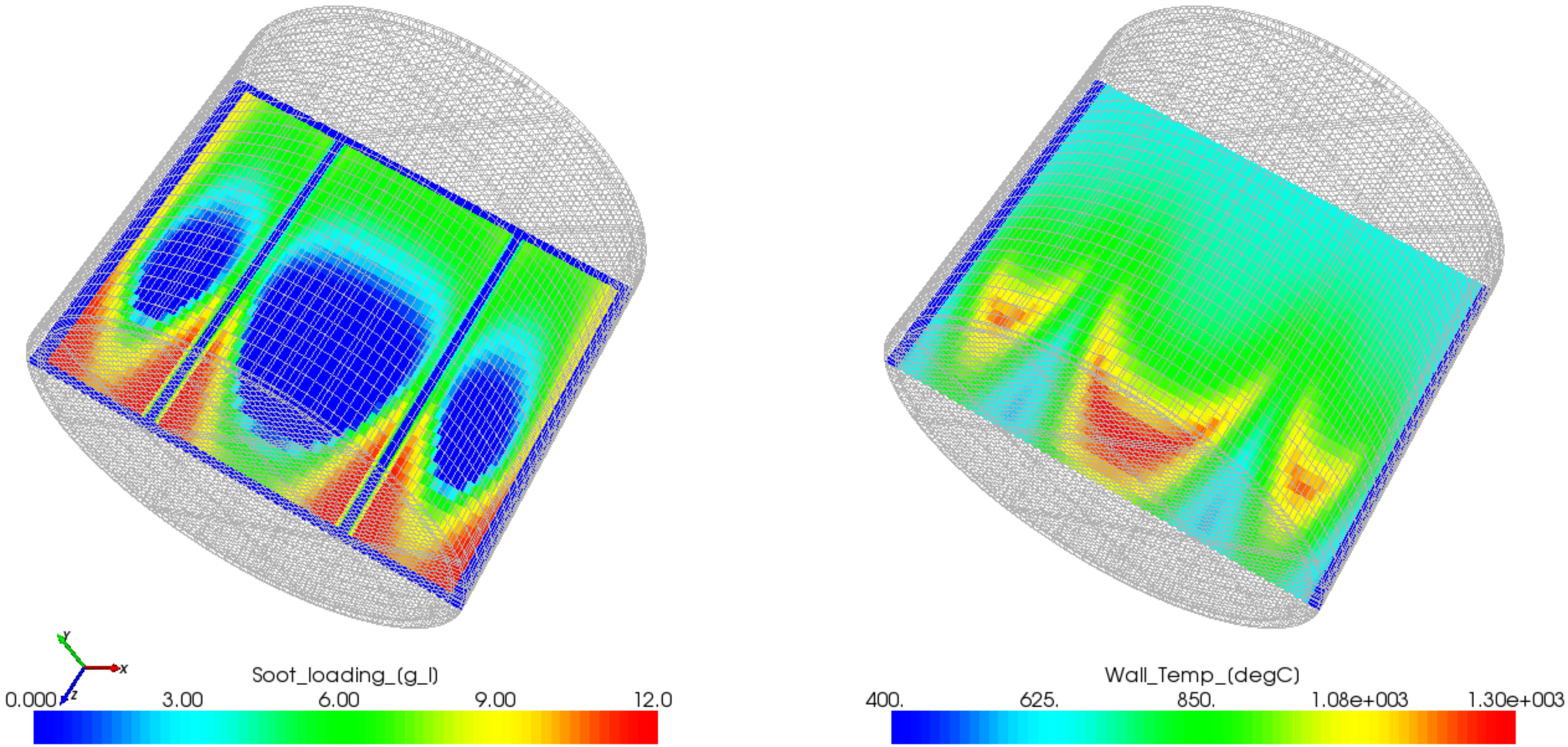




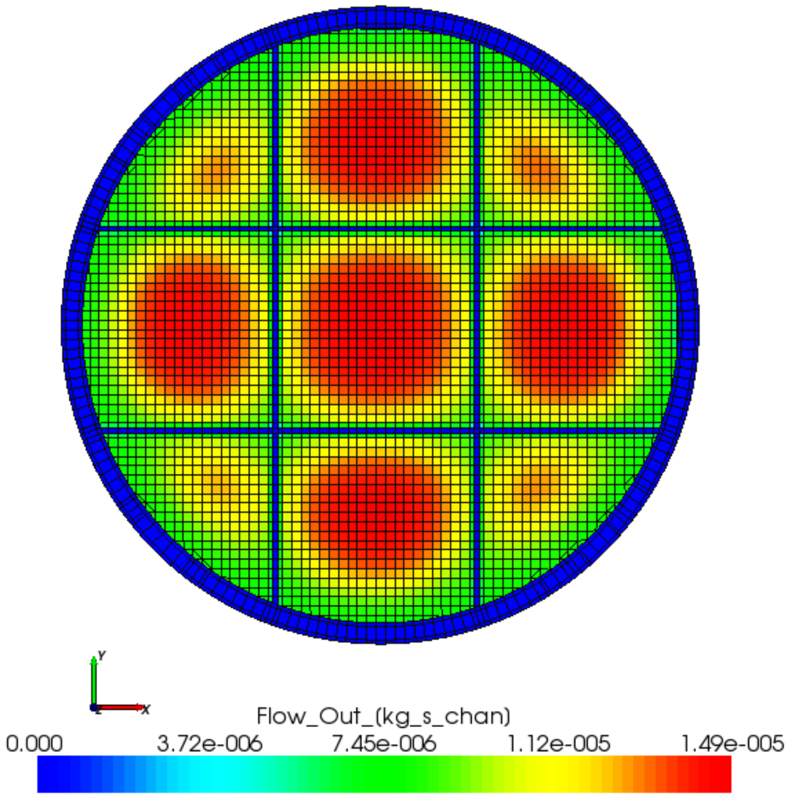


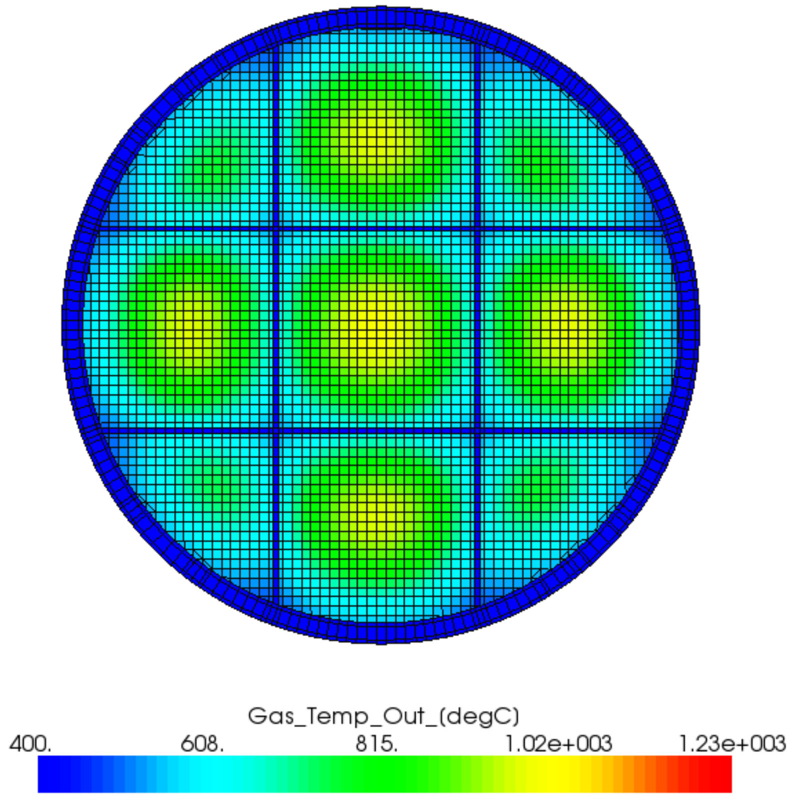
Due to the relatively low flow rate, the temperature increases excessively and the regeneration rates are fast. Highest temperatures near filter exit.

Soot loading and temperature distribution
Initial soot loading: 10.5 g/l

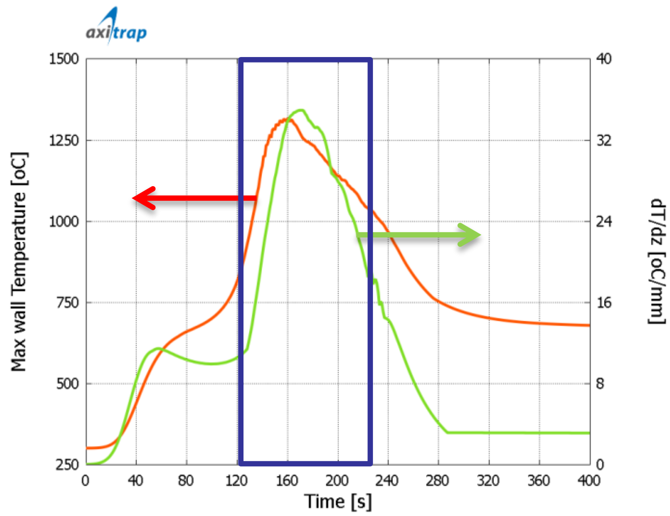


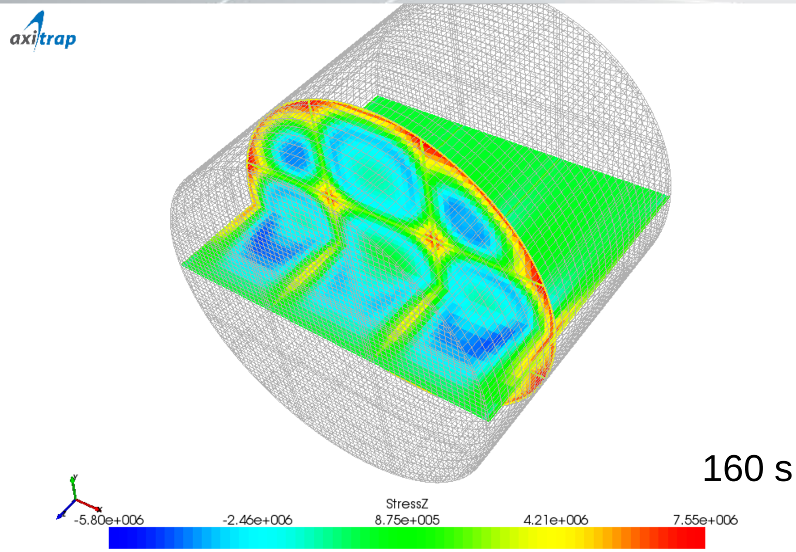
Flow distribution and gas outlet temperature
Initial soot loading: 10.5 g/l

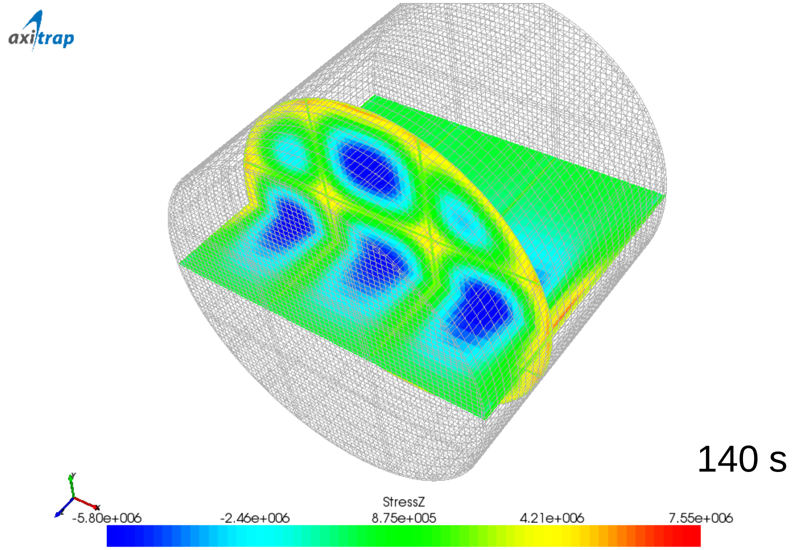


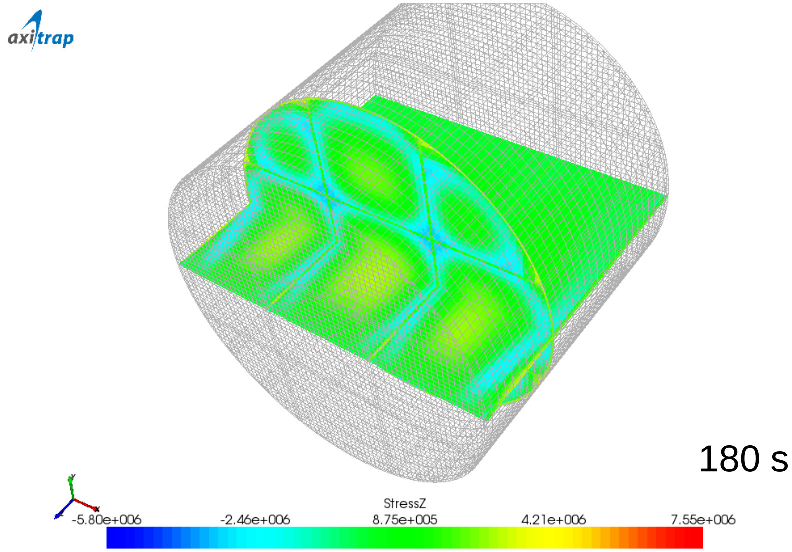


Axial stress analysis results
Initial soot loading: 10.5 g/l

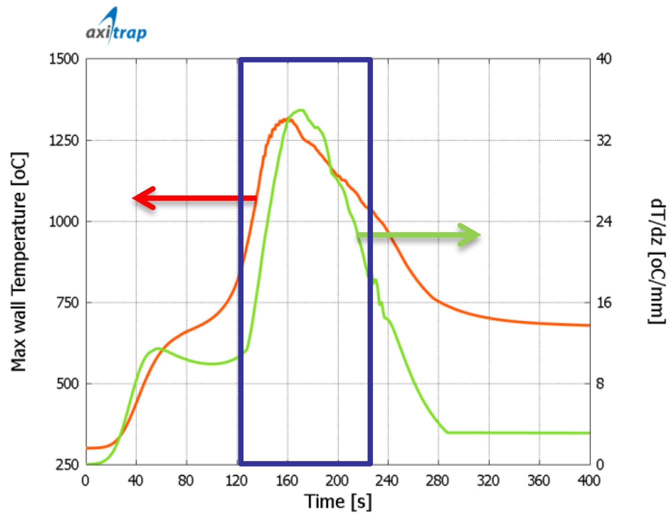


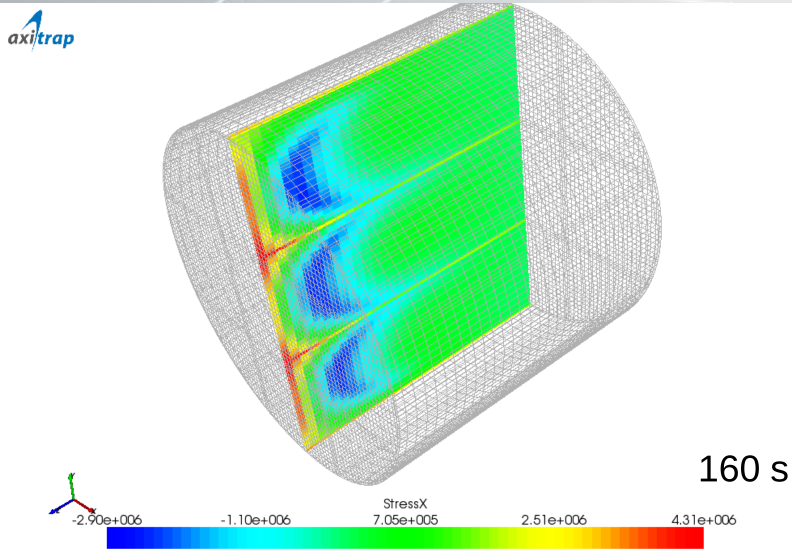


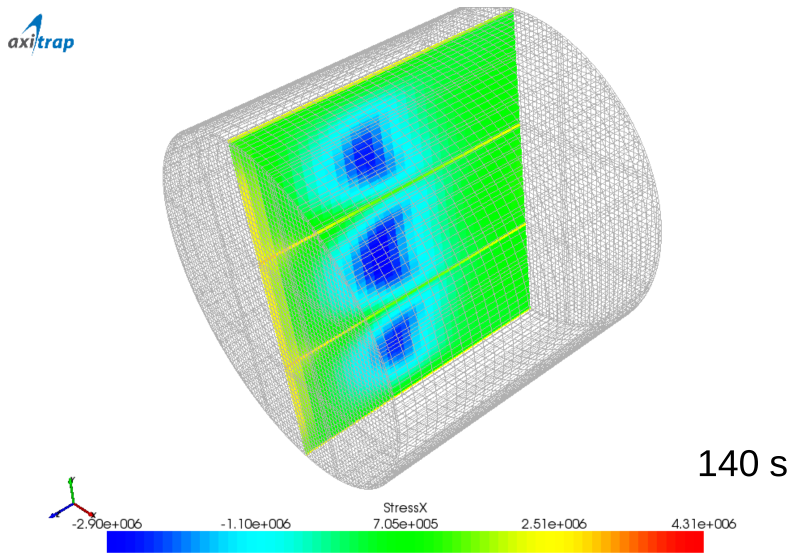


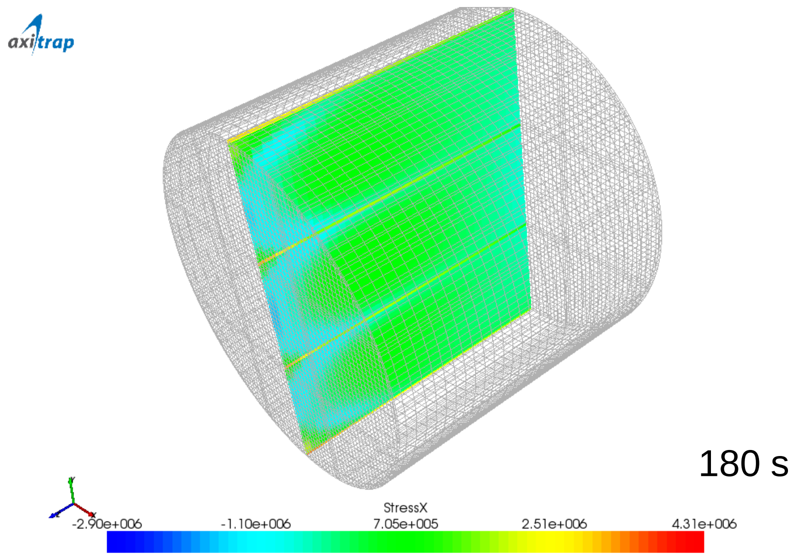


Radial stress analysis results
Initial soot loading: 10.5 g/l



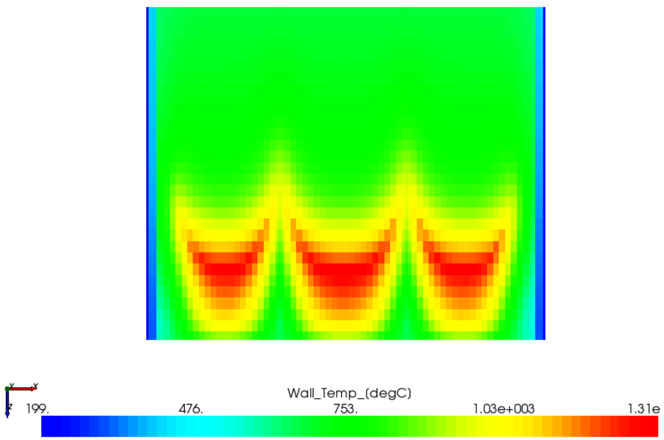




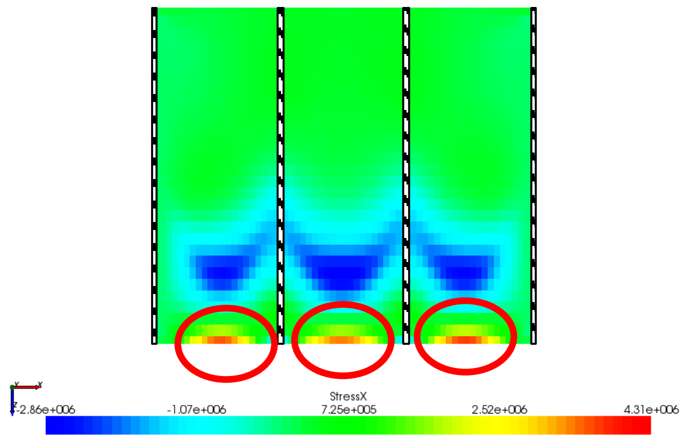


Stress analysis results
Face cracks, ring-off cracks

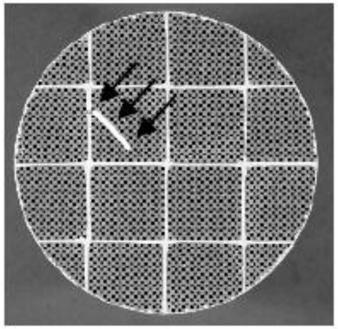
Temperature



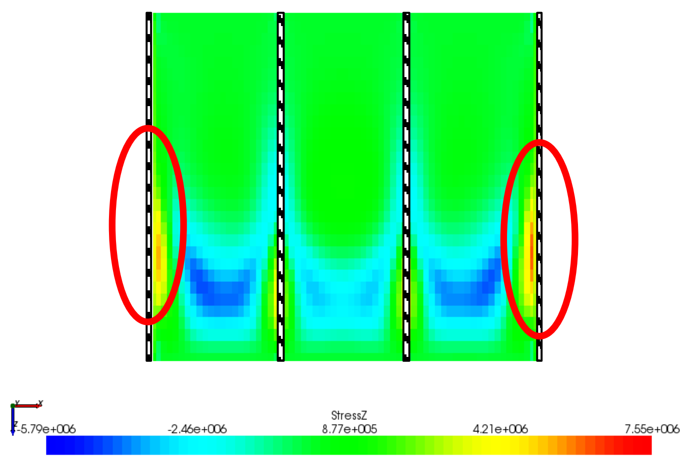
Radial stress



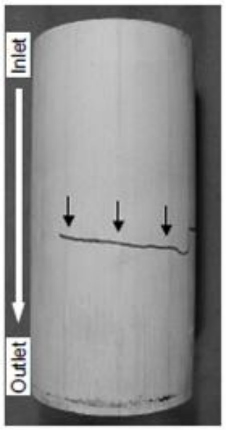
Face crack



Axial stress



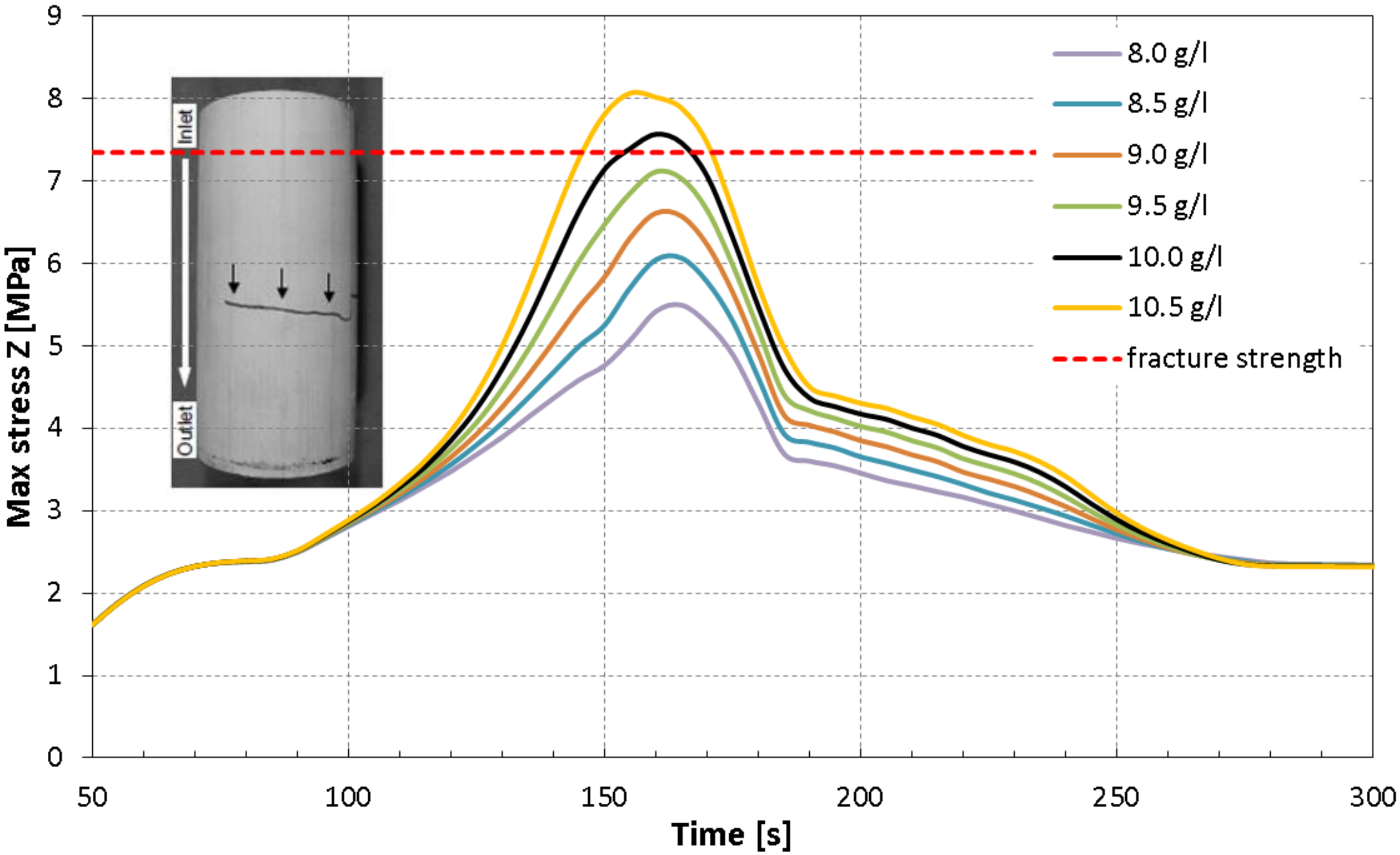
Ring-off crack



Mizutani et al,
SAE 2006-01-1527

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

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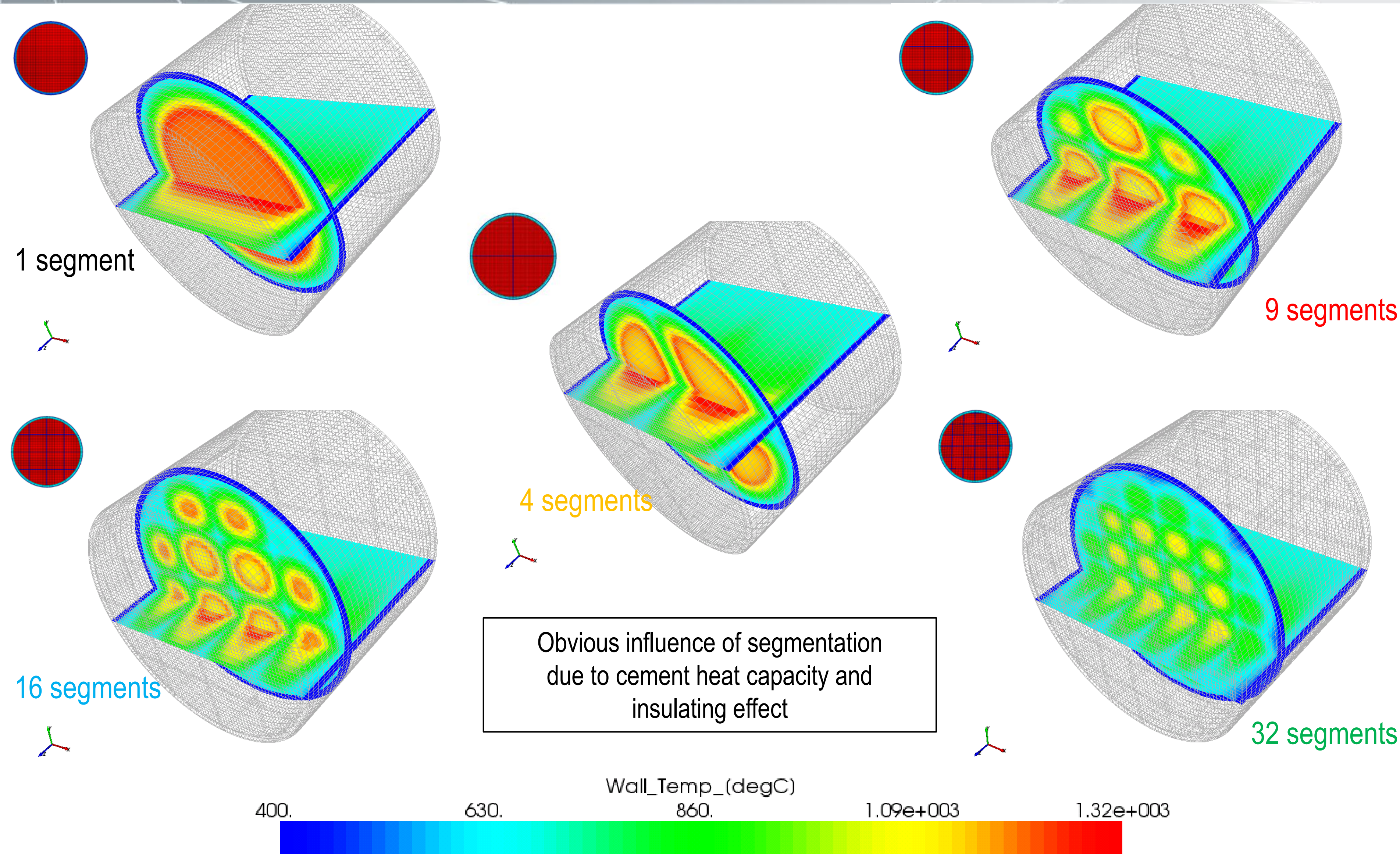
Parametric analysis
Assumptions and parameters varied

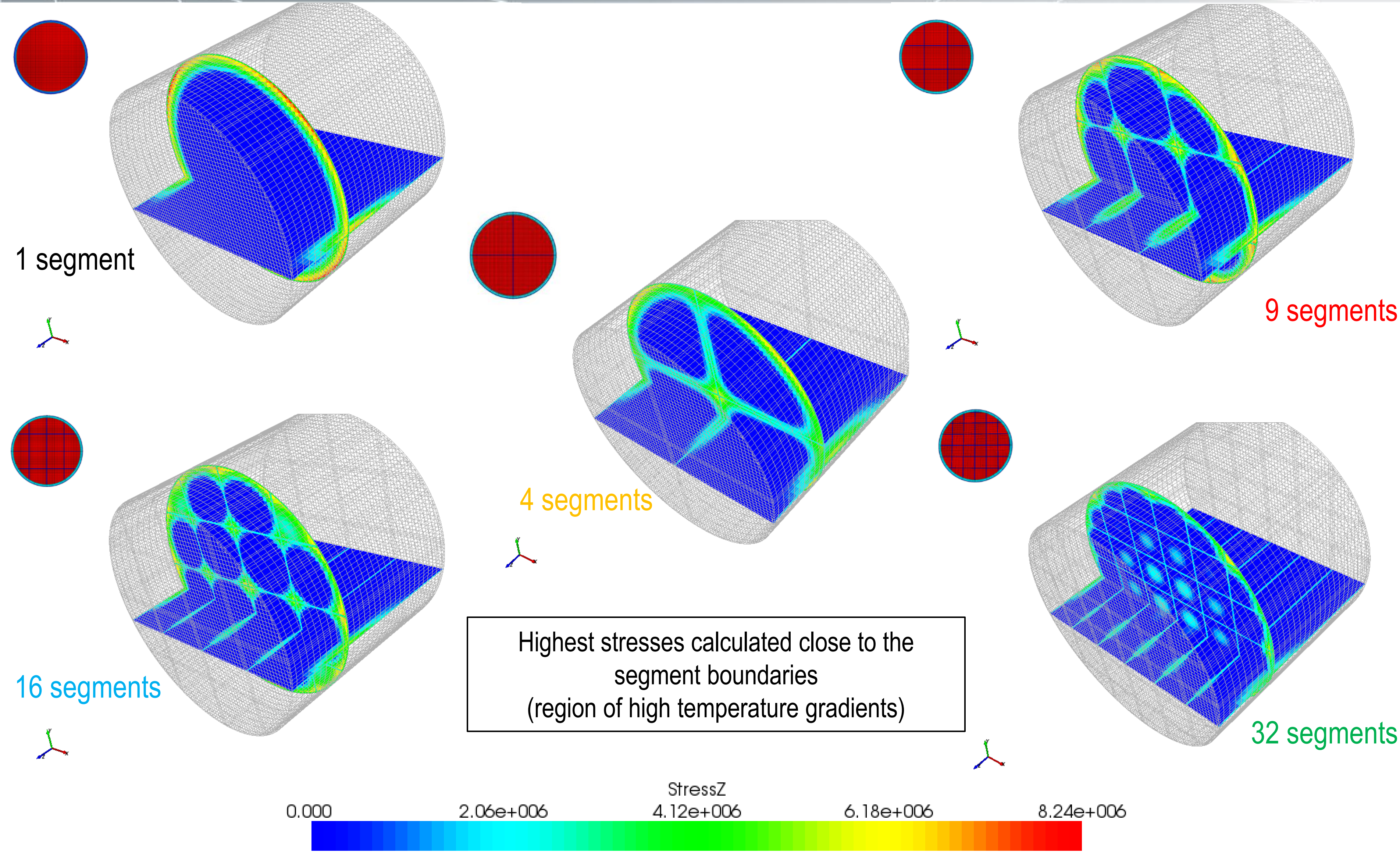
- Parameters kept constant as reference case
  - All inlet gas conditions
  - DOC
  - DPF external dimensions
  - DPF cell structure
  - Initial soot loading
- Parameters varied in the parametric analysis
  - Number of segments
  - Wall porosity: 42% to 70%
  - Cement thermal expansion coefficient: 25% to 400% of baseline value
- The soot mass limit is evaluated for <u>axial</u> stresses only.

Variation of DPF segments: Temperature fields at the occurrence of peak temperature



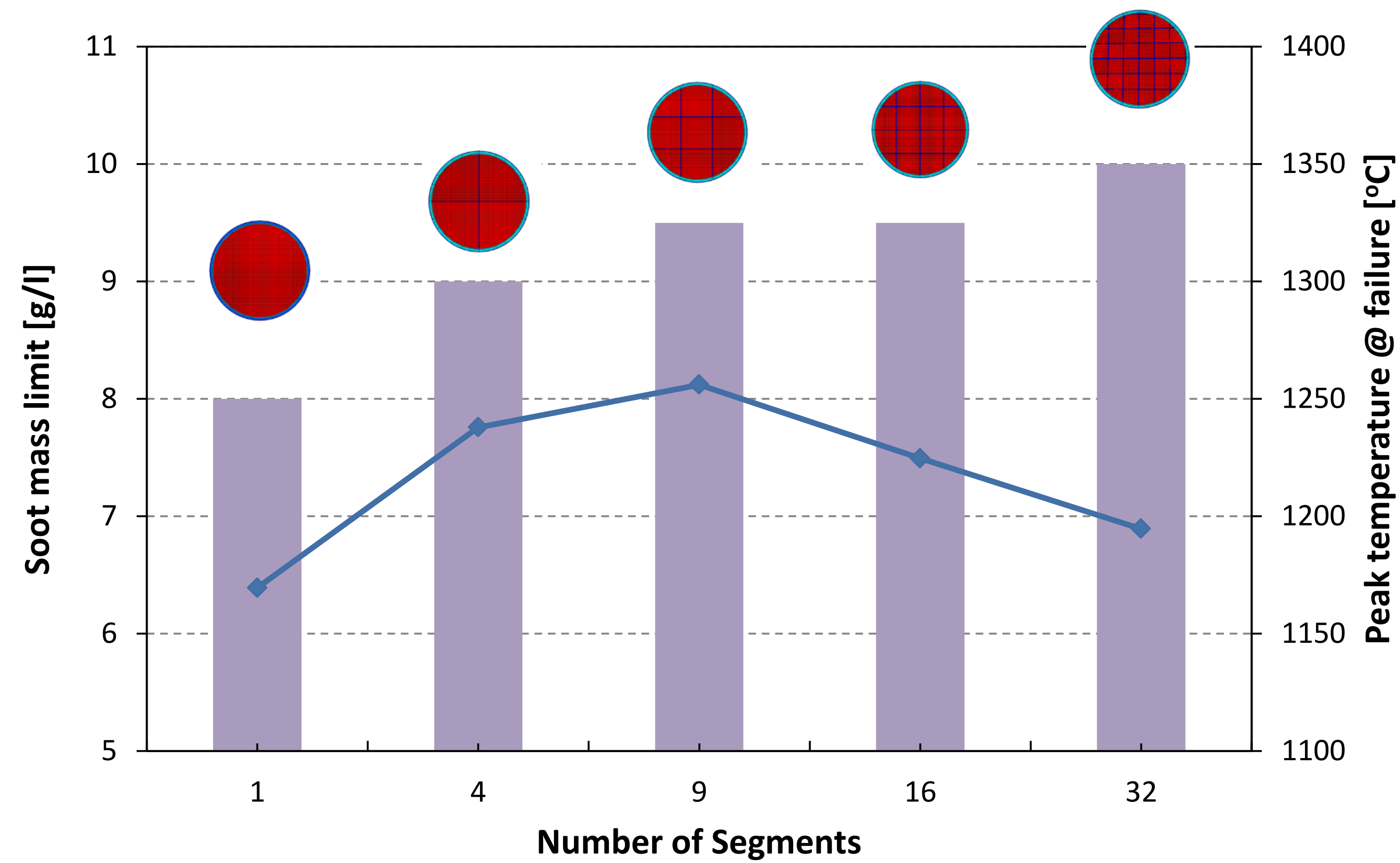
Obvious influence of segmentation due to cement heat capacity and insulating effect

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

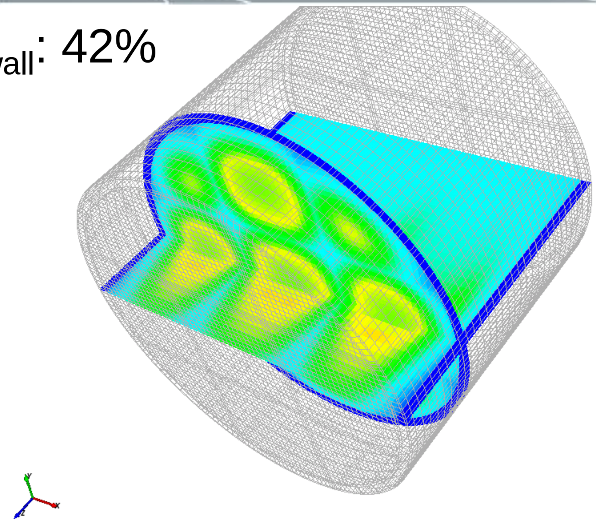
Wall density $\mathrm{d}(\varepsilon) = \mathrm{d}_0(1-\varepsilon)$
Wall conductivity [W/mK] $\mathrm{k}(\varepsilon) = \mathrm{k}_0(1-\varepsilon)$
Young modulus [GPa]: $\mathrm{E}(\varepsilon) = \mathrm{E}_0 \frac{(1-\varepsilon)^2 R}{\varepsilon+(1-\varepsilon) R}$
Fracture strength [MPa] $\sigma(\varepsilon) = \sigma_0 \frac{(1-\varepsilon)^2 R}{\varepsilon+(1-\varepsilon) R}$

ε: porosity
E_0: pore free Young modulus
σ_0: pore free Fracture strength
R: particle size ratio

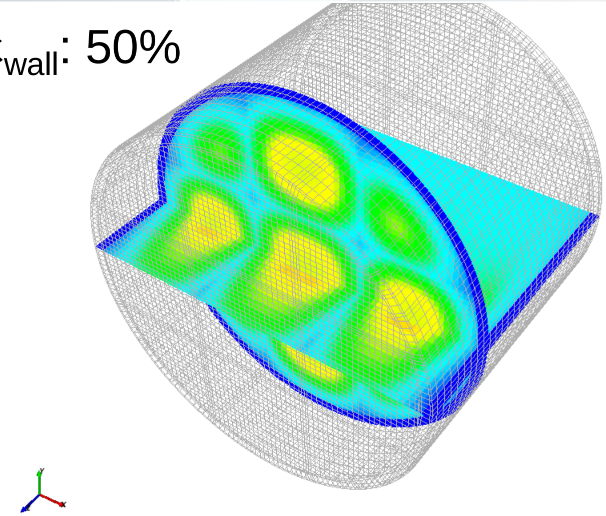
Boccaccini & Fan, Ceram. Int., 1997, Vol 23, p. 239-245

Predicted temperature fields at the occurrence of max stress

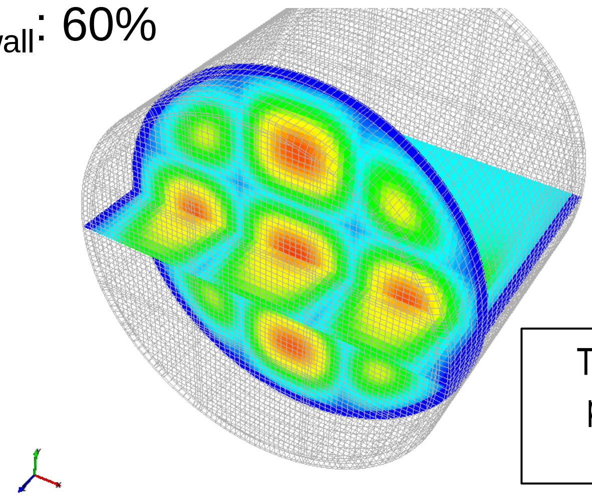
ε_{wall}: 42%



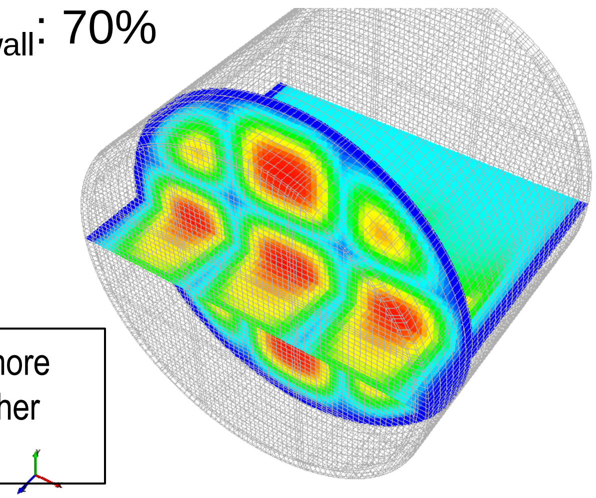
ε_{wall}: 50%



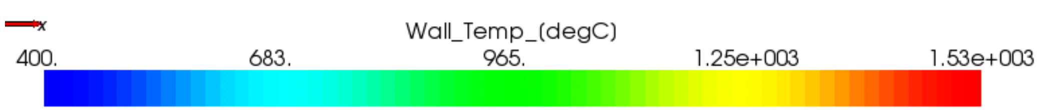
ε_{wall}: 60%



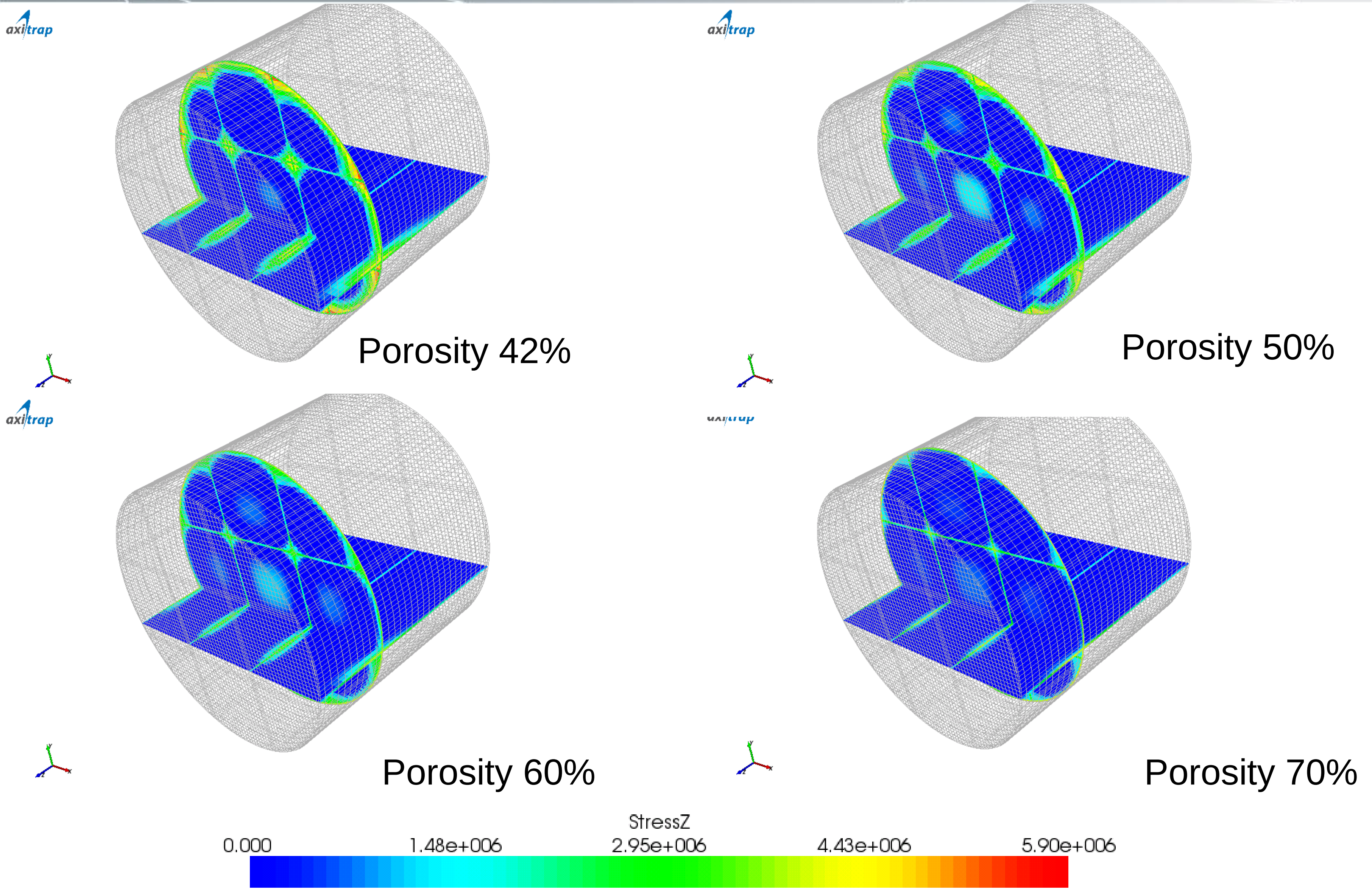
ε_{wall}: 70%



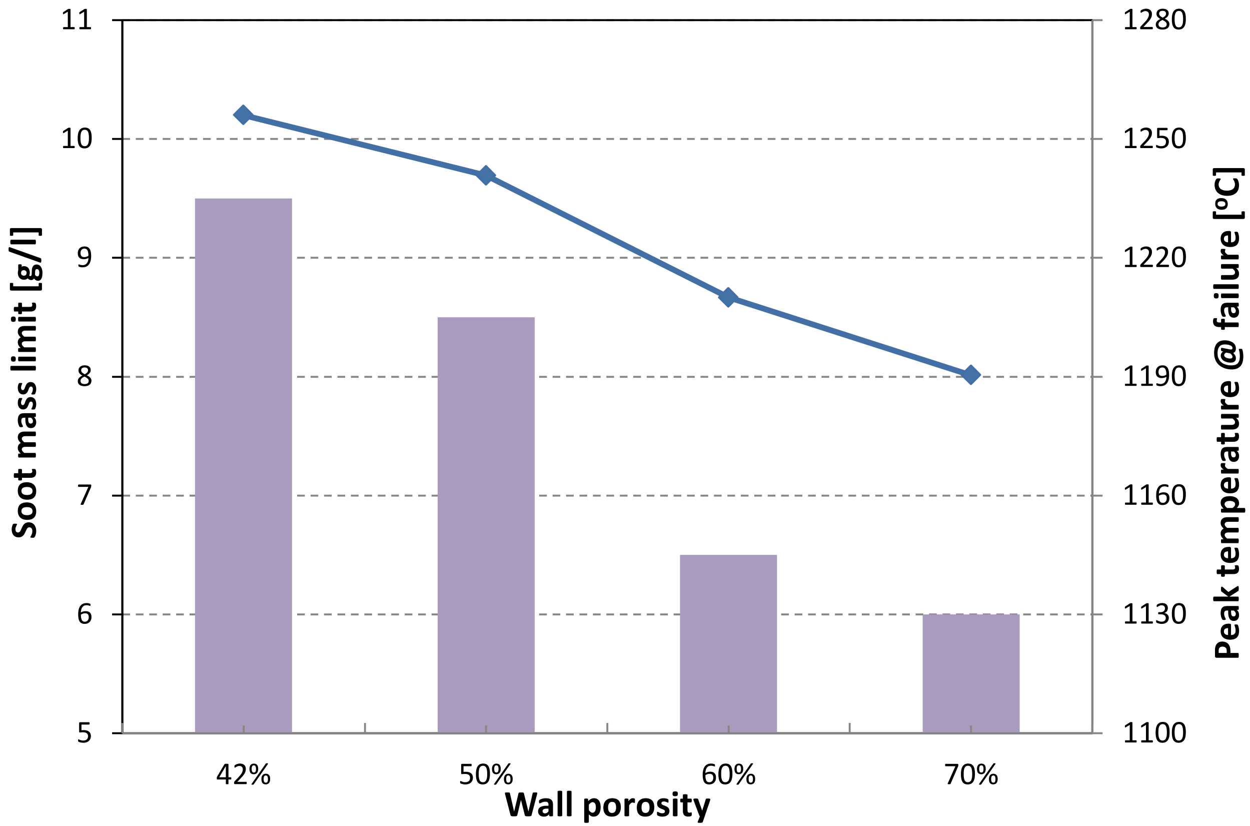
The lower thermal mass of the more porous substrates results to higher temperatures



Axial stress for different wall porosities (9.5 g/l, snapshots at peak stress occurrence)



Soot mass limit vs. wall porosity



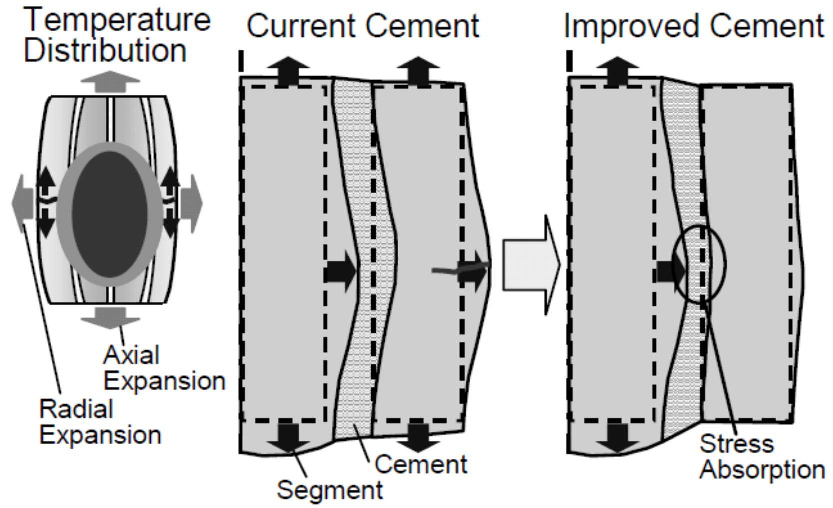
Significant impact of wall porosity on soot mass limit.
Mechanical failure not directly correlated to max. wall temperature
Porosity optimization is subject to additional factors: filtration, pressure drop, coating etc

Cement thermal expansion coefficient variation

Exothermia

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

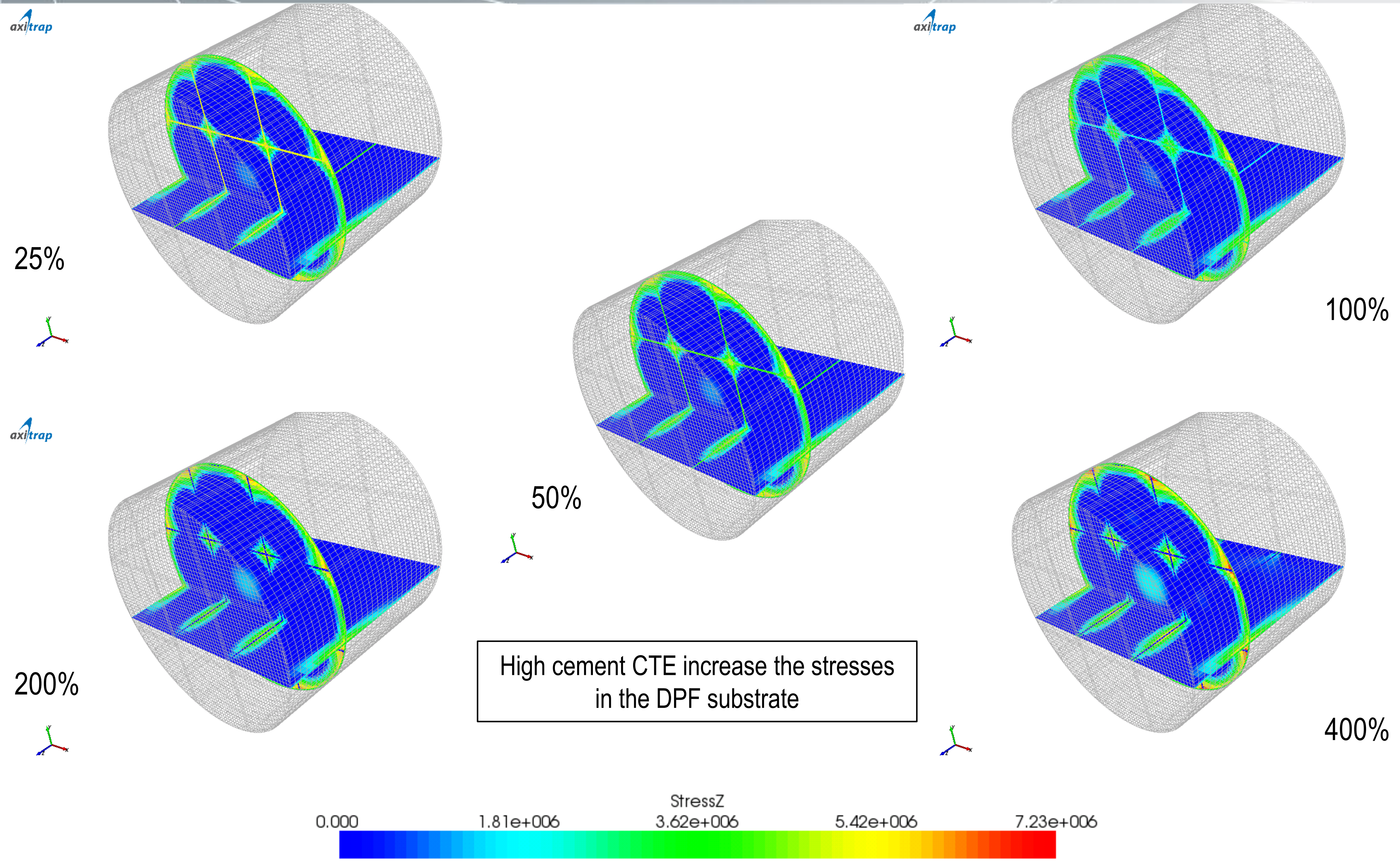


Mizutani et al, SAE paper 2006-01-1527

Cement thermal expansion coefficient [1/K]	400% 200% 100% 50% 25%	$1.08\ 10^{-05}$ $5.40\ 10^{-06}$ $2.70\ 10^{-06}$ $1.35\ 10^{-06}$ $6.75\ 10^{-07}$

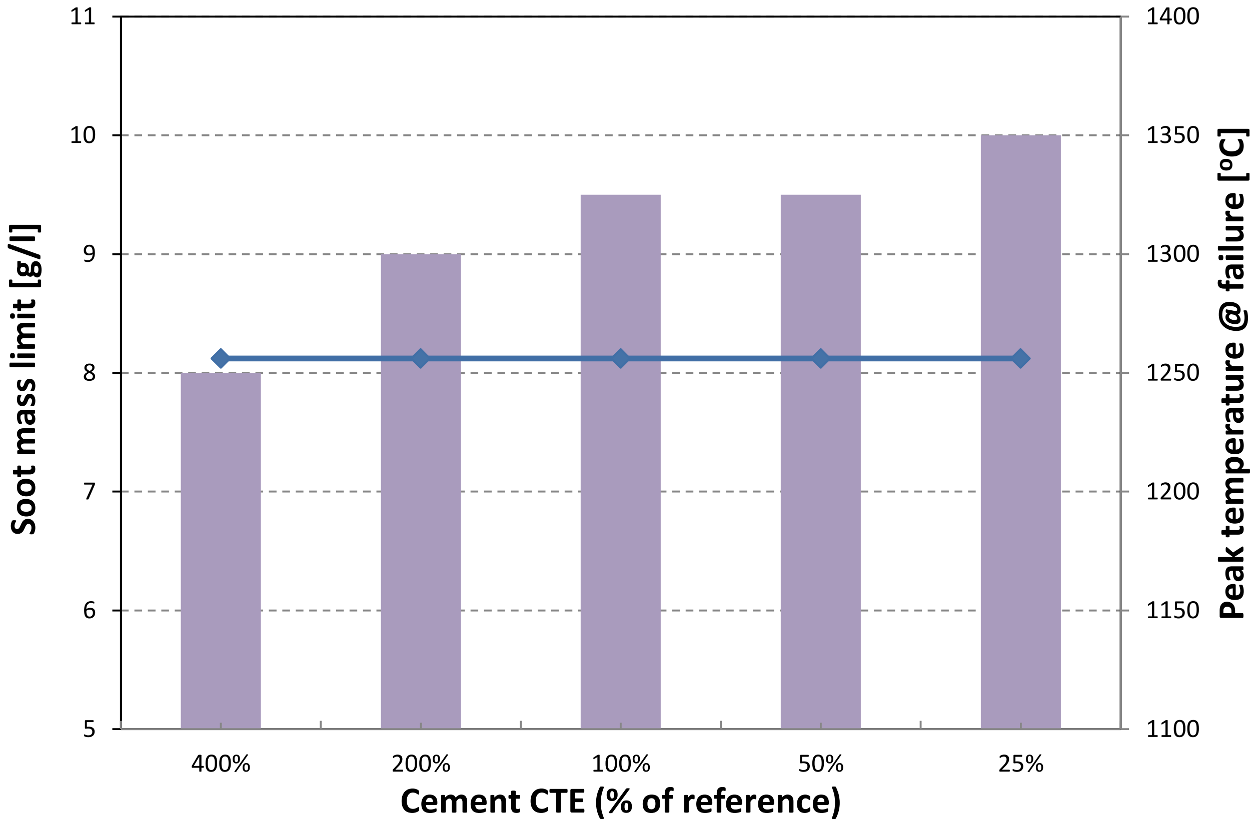
Axial stresses for different cement TCE. 9.5 g/l, peak stress occurrence

Exothermia



High cement CTE increase the stresses in the DPF substrate

Soot mass vs. Cement thermal expansion coefficient



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.

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Thank you for your attention!

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