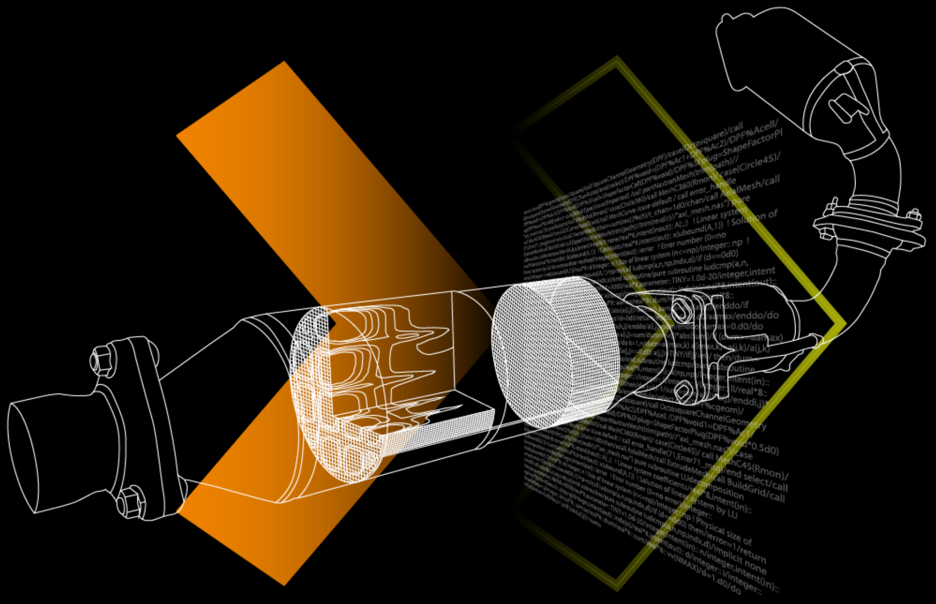

Transient flow and chemistry predictions in exhaust after-treatment systems

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Exothermia S.A.

4th Meeting on ICEngine Simulations Using OpenFOAM(R) Technology 13/02/2020

Outline

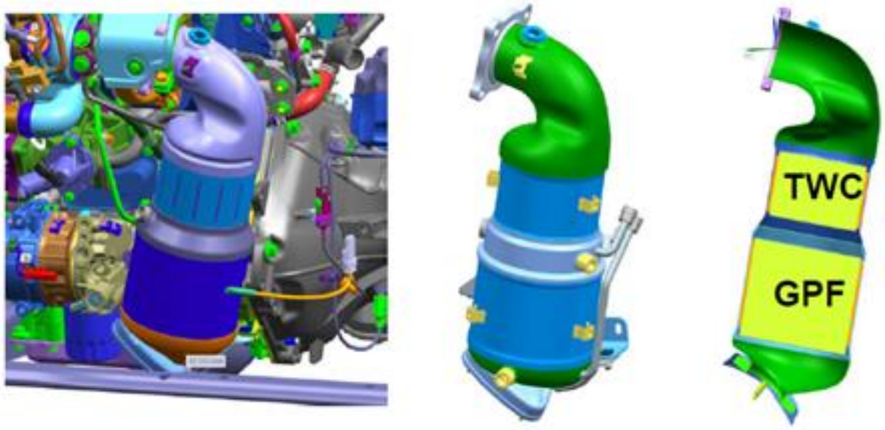
- Motivation
- CFD in exhaust after-treatment systems
- Exothermia/OpenFOAM model description
- Results
  - Cold start
  - DTI
  - Driving cycle
- Conclusions

Motivation

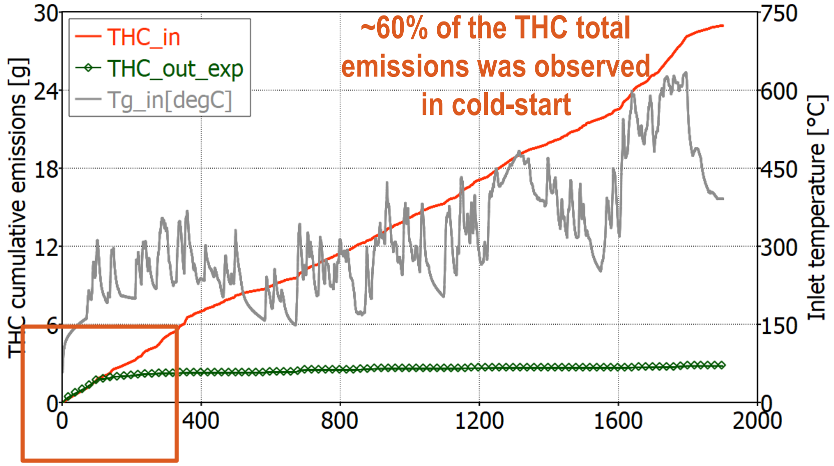
Conventional EAT simulations:

- Usually 1D simulations considering uniform inlet conditions
- 2D simulations taking into account axi-symmetric flow and temperature profile

But lately there are several cases where **flow**, **temperature and species non-uniformities** play an important role at the exhaust after-treatment systems.



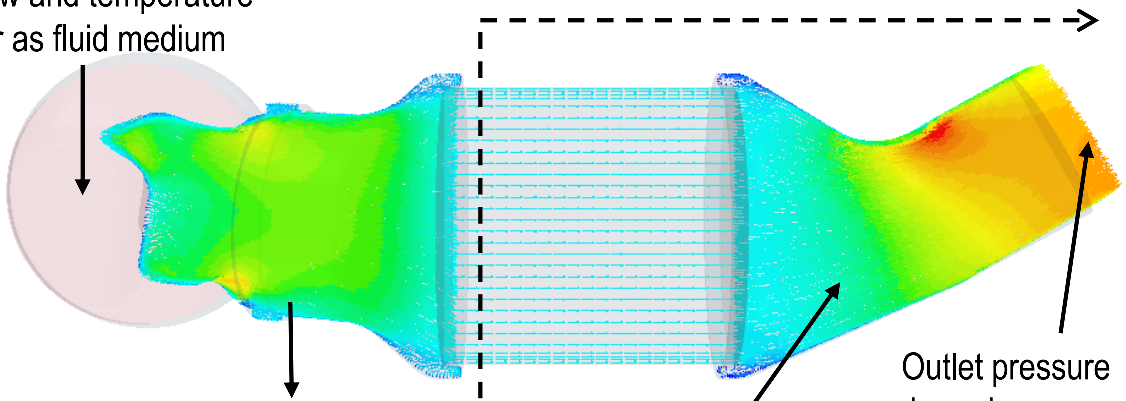
Exhaust components close to engine



Cold start emissions TWC

Traditional CFD approaches

- Steady state simulations at specific engine operating points or “short-time” simulations
- Constant boundary conditions
- Reactions are neglected
- Piping walls are neglected
- Usually, geometry optimization is performed by the uniformity index



Inlet boundary:

- Constant inlet mass flow and temperature
- Air as fluid medium

Wall boundaries:

- Heat losses:
  Resistance = 0.02 m² °C / W
  Ambient temperature = 27 °C

Wall boundaries:

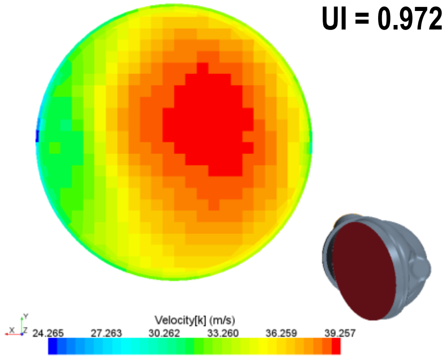
- Adiabatic

Outlet pressure boundary:

- Pressure difference: 0 Pa

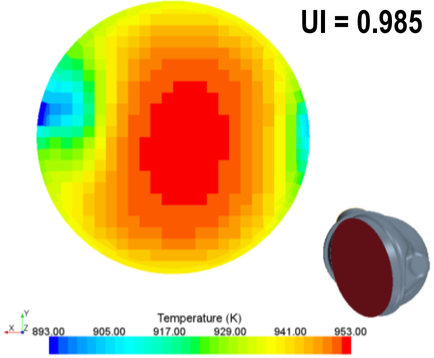
Velocity

UI = 0.972



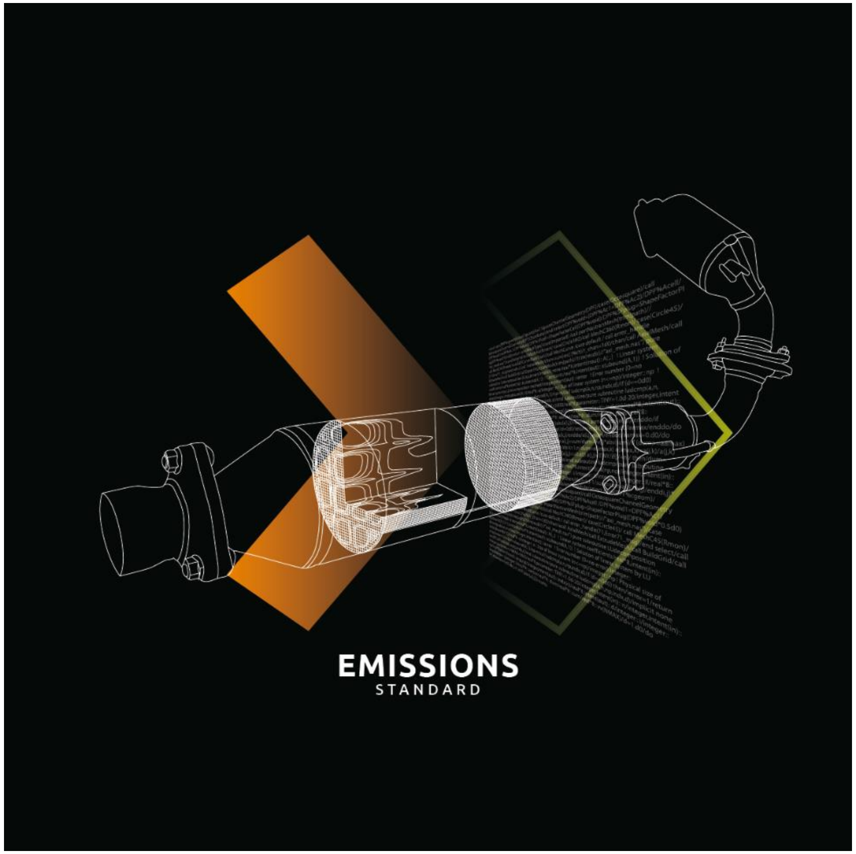
Temperature

UI = 0.985

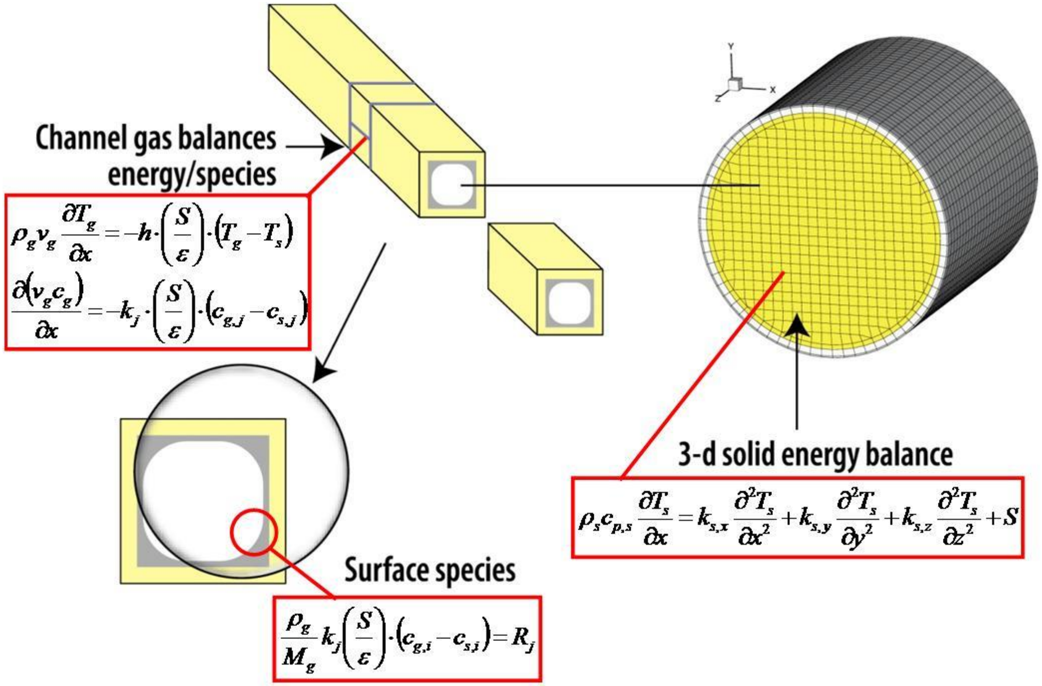


Exothermia suite

- The industry benchmark in exhaust system simulation
  - unparalleled level of scientific depth
  - continuous validations vs real-world tests.
- Modeling of exhaust components for gasoline, Diesel, CNG engines
  - Catalysts
  - Filters
  - Auxiliary components (sensors, injectors, mixers, thermoelectric generators etc).



TWC 3d+2d reactor model
Balance equations & reactions



Channel gas balances energy/species

$$\rho_g v_g \frac{\partial T_g}{\partial x} = -h \cdot \left(\frac{S}{\varepsilon}\right) \cdot \left(T_g - T_s\right)$$

$$\frac{\partial\left(v_g c_g\right)}{\partial x} = -k_j \cdot \left(\frac{S}{\varepsilon}\right) \cdot \left(c_{g,j} - c_{s,j}\right)$$

3-d solid energy balance

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

Surface species

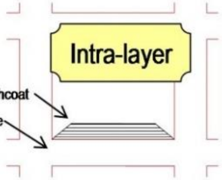
$$\frac{\rho_g}{M_g} k_j \left(\frac{S}{\varepsilon}\right) \cdot \left(c_{g,i} - c_{s,i}\right) = R_j$$

1. CO + 1/2 O2 --> CO2
2. H2 + 1/2 O2 --> H2O
3. CH4 + 2 O2 --> CO2 + 2 H2O
4. C3H6 + 9/2 O2 --> 3 CO2 + 3 H2O

5\. C3H6 + 9 NO --> 3 CO2 +3 H2O + 9/2 N2
6\. CO + 2 NO --> CO2 + N2O
7\. H2 + 2 NO --> H2O + N2O
8\. NO + 5/2 H2 --> NH3 + H2O

5\. NO + 5/2 CO +3/2 H2O --> NH3 + 5/2 CO2
6\. N2O + CO --> N2 + CO2
7\. N2O + H2 --> N2 + H2O
8\. NH3 + 3/2 NO --> 5/4 N2 + 3/2 H2O

5\. fCe2O3 + 1/2 O2 --> 2 fCeO2
6\. fCe2O3 + NO --> 2 fCeO2 + 1/2 N2
7\. 2 fCeO2 + CO <--> fCe2O3 + CO2
8\. 2 fCeO2 + H2 <--> fCe2O3 + H2O
9\. 2 fCeO2 + 1/6 C3H6 --> fCe2O3 + 1/2 CO + 1/2 H2O
18\. Ce2O3 + 1/2 O2 --> 2 CeO2
19\. Ce2O3 + NO --> 2 CeO2 + 1/2 N2
20\. 2 CeO2 + CO --> Ce2O3 + CO2
21\. 2 CeO2 + H2 --> Ce2O3 + H2O
22\. 2 CeO2 + 1/6 C3H6 --> Ce2O3 + 1/2 CO + 1/2 H2O



Washcoat:

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

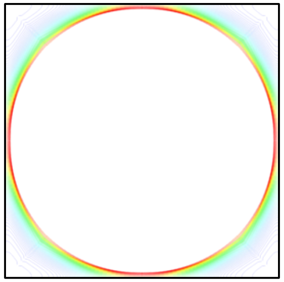
Channel gas species balance:

$$\frac{\partial}{\partial z}\left(v_1 y_{1,j}\right) = \frac{1}{df_{-w}} k_{1,j}\left(y_{1s,j} - y_{1,j}\right), \qquad k_{i,j} = \frac{Sh \cdot D_{mol,j}}{d_i}$$

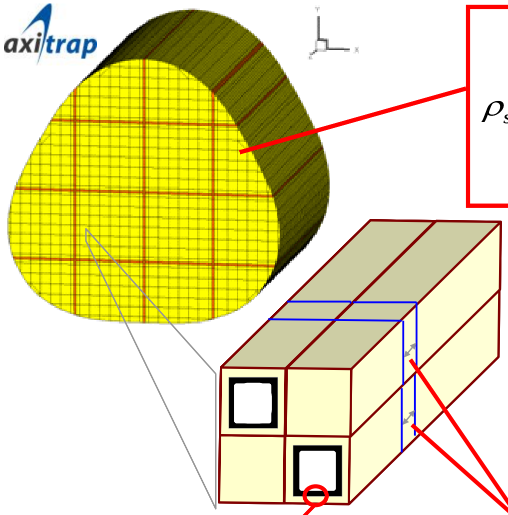
Boundary conditions:

$$-D_j f_{-w} \left.\frac{\partial y_j}{\partial x}\right|_{1s} = -df_{-w}{}^2 \frac{\partial}{\partial z}\left(v_1 y_{1,j}\right), \qquad \left.\frac{\partial y_j}{\partial x}\right|_{2s} = 0$$

Variable thickness coating



GPF 3d+1d reactor model
Balance equations & reactions



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

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

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

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

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

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

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

Wall/soot scale balances
Momentum/soot/ species

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

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

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

1. CO + 1/2 O2 --> CO2
2. H2 + 1/2 O2 --> H2O
3. CH4 + 2 O2 --> CO2 + 2 H2O
4. C3H6 + 9/2 O2 --> 3 CO2 + 3 H2O

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21. 2 CeO2 + H2 --> Ce2O3 + H2O
22. 2 CeO2 + 1/6 C3H6 --> Ce2O3 + 1/2 CO + 1/2 H2O

Combining CFD + Exothermia suite

CFD

- **Detailed complex geometry representation**
- **Effective solution for**:
  - flow field
  - flow/temperature/species non-uniformities
  - energy balance

exothermia

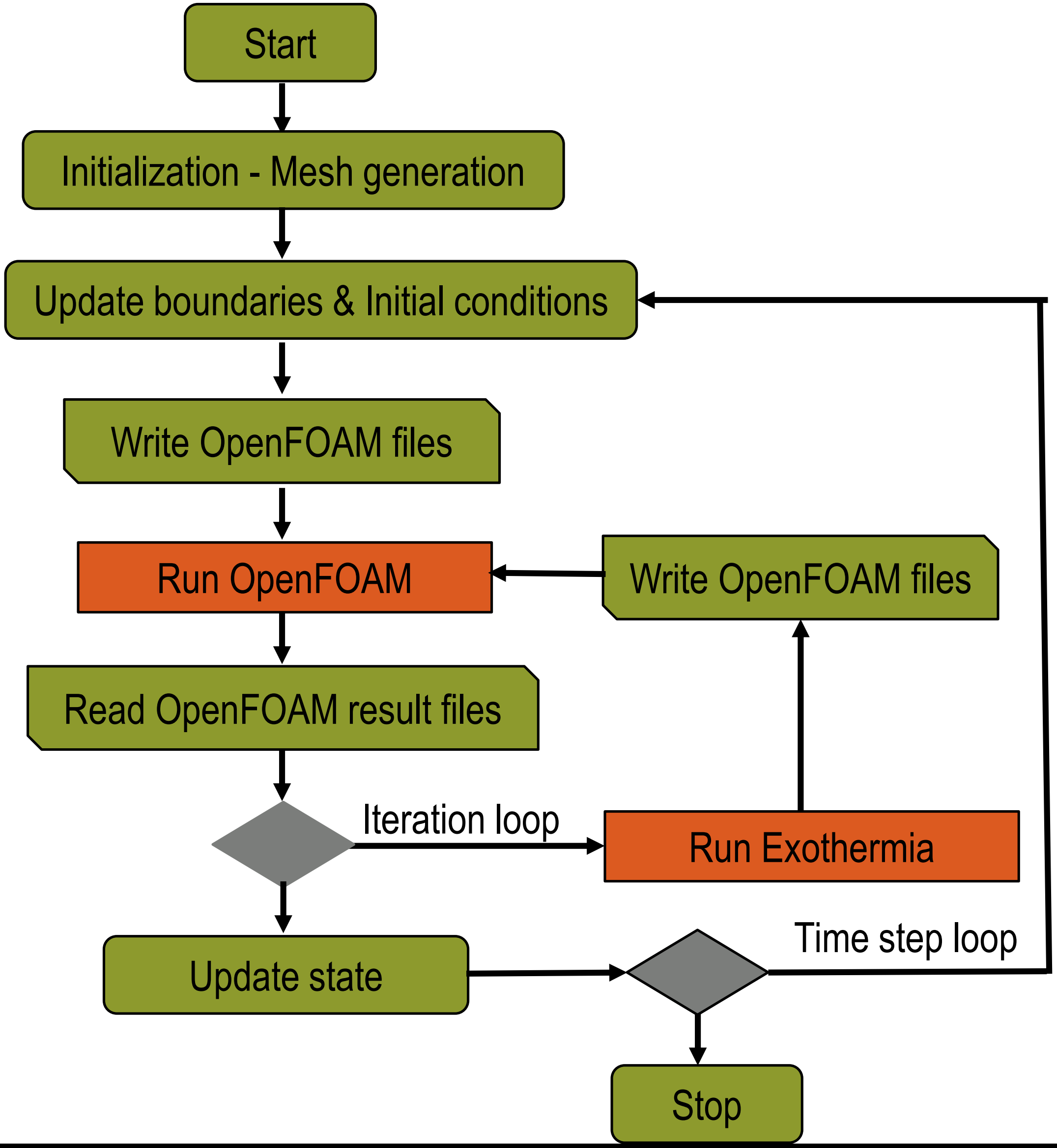
- **Detailed device structure representation** (porosity, channels, washcoat, etc.)
- **Detailed chemistry models**
- **Detailed filtration models**
- **Detailed heat/mass transfer models**
- **Fast and reliable complex reactor modeling**

Coupling combines the benefits of both worlds and is useful when the catalytic reactor is packaged in ways that do not guarantee evenly distributed flow, temperature and species at its entrance

› Why OpenFOAM?

- Wide range of application and models
- Seamless integration
- Automatic parallelization
- No license costs

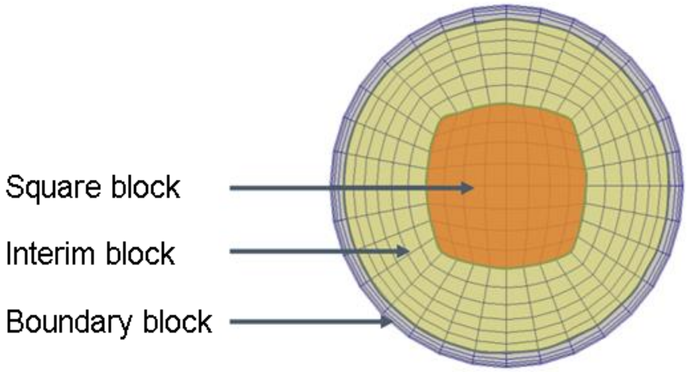
Coupling algorithm

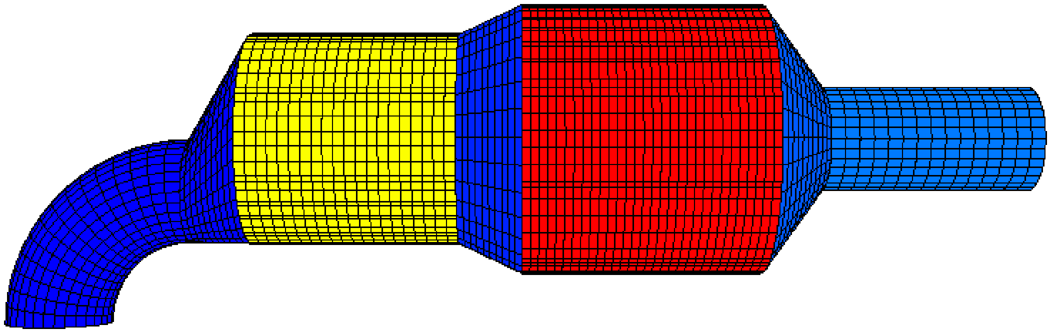


- Automatic in-house meshing
- Boundary & initial conditions via the Exothermia GUI
- Smart algorithm for optimal initial conditions
- OpenFOAM solver runs in steady state mode
- Data exchange using files

Mesh generation algorithm

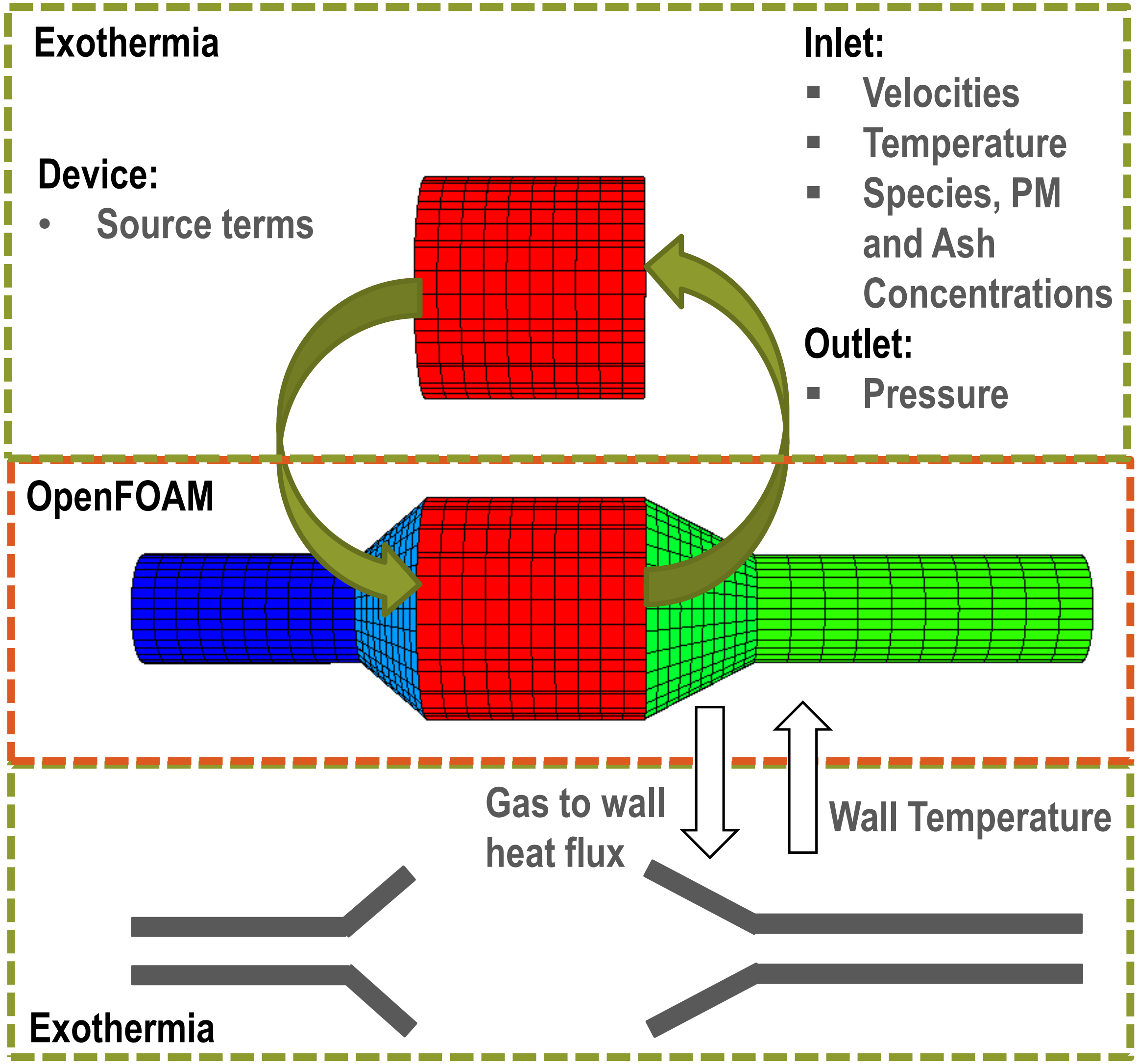
- In-house geometry and mesh algorithm
- Easy configuration
- Support of straight and bent pipes
- Support of eccentric and tilted cones





Data exchange
Monolith and duct

- Data exchange at every iteration till convergence
- **Exhaust gas**: Exothermia gets from OpenFOAM the necessary distributions and calculates the respective source terms based on monolith parametrization
- **Confining walls:** Exothermia gets from OpenFOAM the heat flux and calculates the respective wall temperature



Exothermia

Device:

- Source terms

Inlet:

- Velocities
- Temperature
- Species, PM and Ash Concentrations

Outlet:

- Pressure

OpenFOAM

Gas to wall heat flux

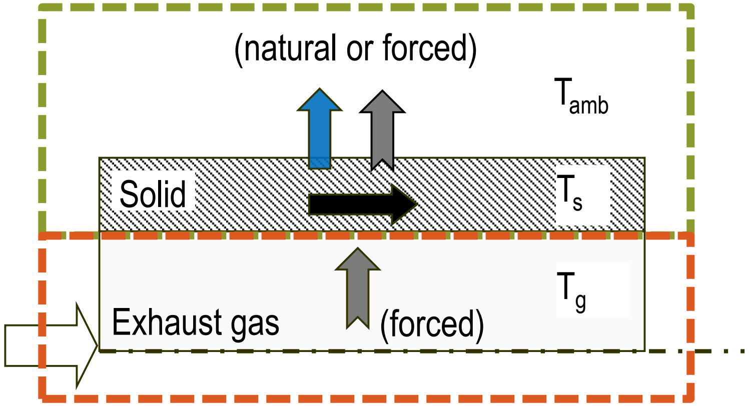
Wall Temperature

Exothermia

Transient wall boundary condition

➡ Conduction
➡ Convection
➡ Radiation
🟩 Exothermia
🟧 OpenFOAM

Single wall pipe



Solid energy balance

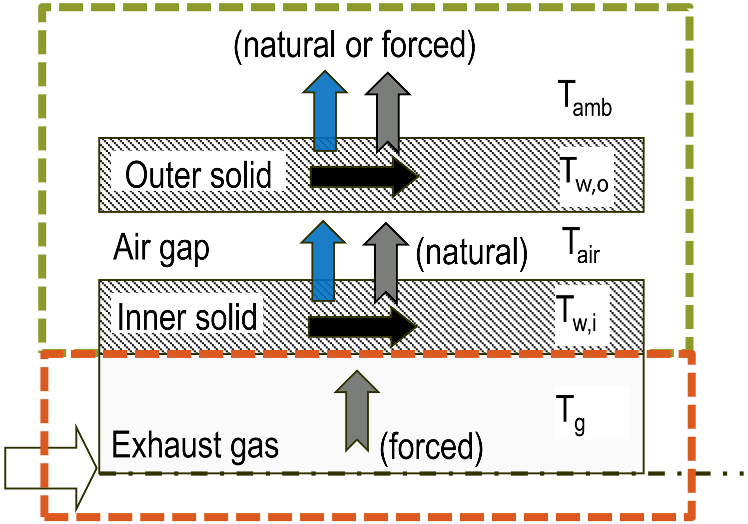
$$\rho_S\, C_{p,S} \frac{\partial T_S}{\partial t} = \boxed{\lambda_S \frac{\partial^2 T_S}{\partial z^2} + \lambda_S \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial T_S}{\partial r}\right)} + S$$

Solid boundary conditions

$$\lambda_{S,r}\frac{\partial T_S}{\partial r} = \boxed{C_{amb}\, h_{amb}(T_S - T_{amb})} + \boxed{C_{rad}\, \varepsilon_{rad}\, \sigma\left({T_S}^4 - {T_{amb}}^4\right)}$$

$$\rho_g\, C_{p,g}\, u_g \frac{\partial T_S}{\partial r} = \boxed{S_{gas \to solid}}$$

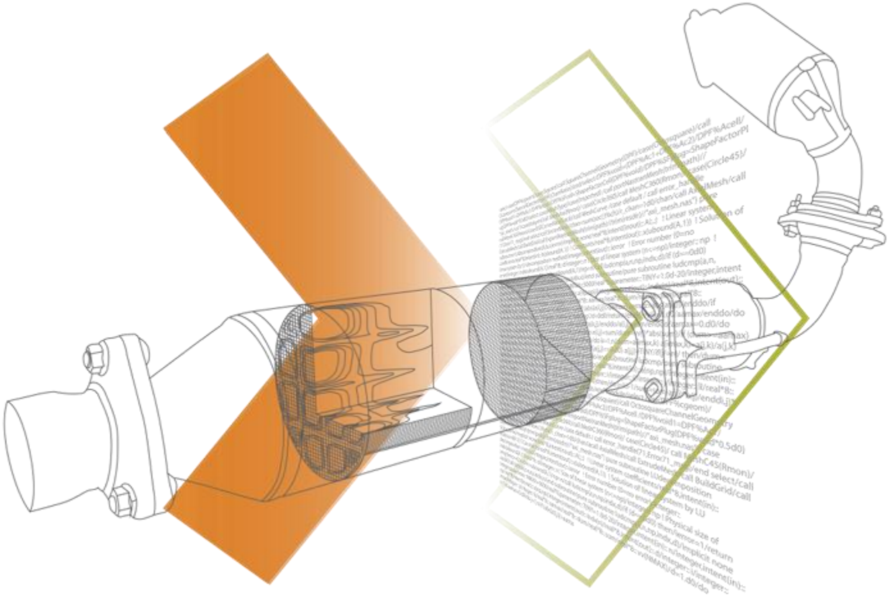
Double wall pipe with air gap



Inner solid boundary condition

$$\lambda_{S,r}\frac{\partial T_S}{\partial r} = \boxed{h_{gap}\left(T_{w,o} - T_{w,i}\right)} + \boxed{q_{rad,gap}}$$

exothermia
EFFICIENCY. PREDICTED.

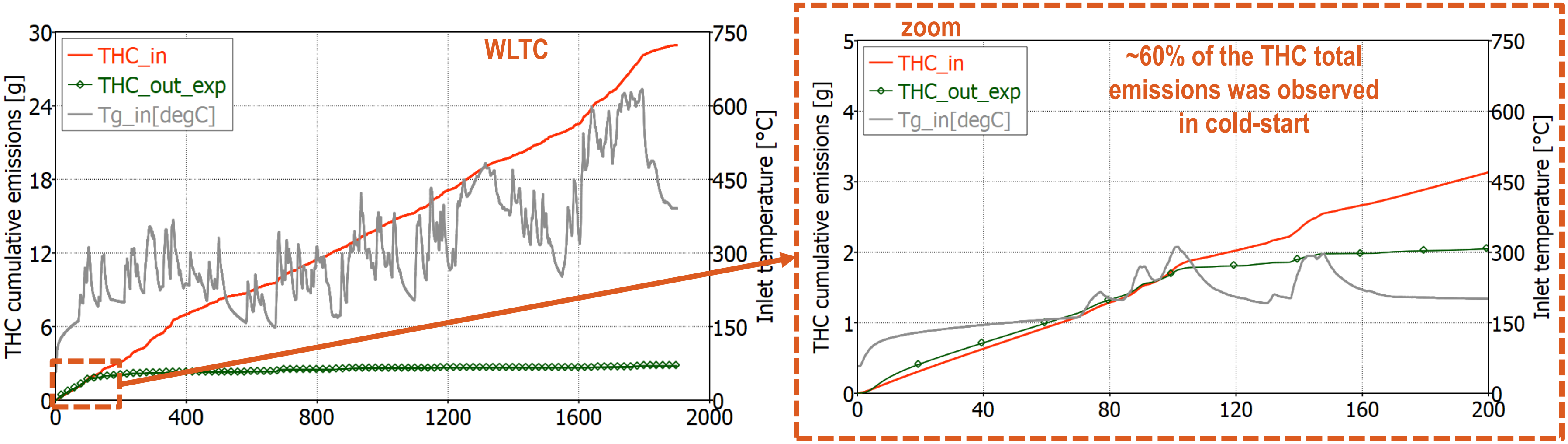


Cold-start

Cold-start issue

Cold start: The starting of a vehicle engine at a low temperature relative to its operating temperature.

- Catalytic converters used for after-treatment systems operate when their temperature reaches a certain threshold, the so-called light-off temperature (200-250°C for TWC).
- Hybrid Electric Vehicle (HEV) engines are usually switched off at low speed and wheel torque which leads to reduction of the exhaust temperature, and thus cold start problem becomes great issue for the catalyst efficiency.


WLTC

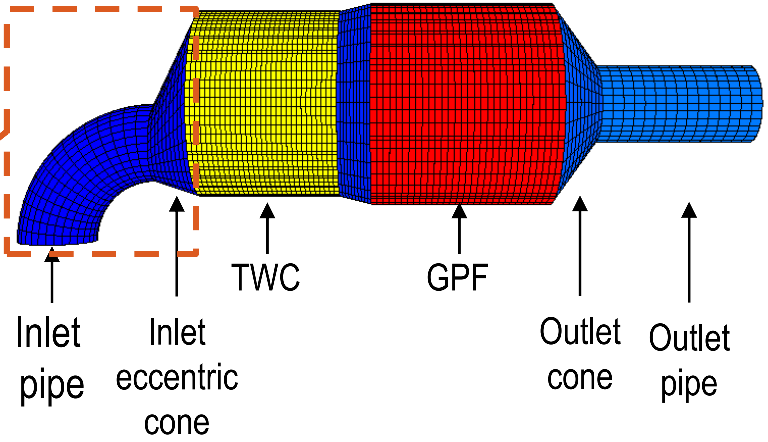
zoom

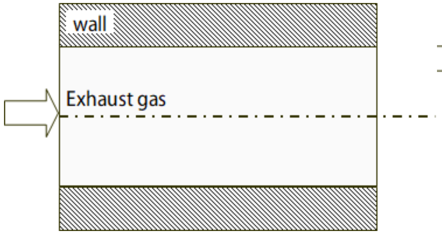
~60% of the THC total emissions was observed in cold-start

- High percentage of the emissions for the legislated pollutants (CO, THC, NOx) are emitted during engine cold-start and warm-up period.

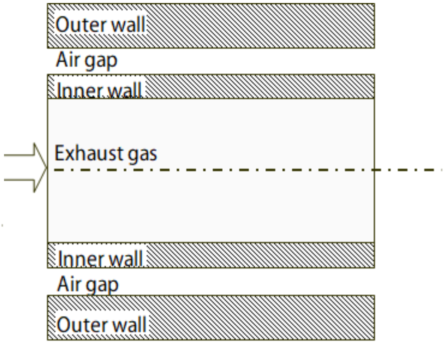
Problem statement

- **Problem description**: Two inlet pipe and cone setups will be investigated for their affect on the species conversion efficiency during cold start period
  - Case1: Single wall pipe
    - 1.5mm wall
  - Case 2: Dual wall with airgap
    - 0.3mm inner wall
    - 3.0mm airgap
    - 1.5mm outer wall





Single wall pipe

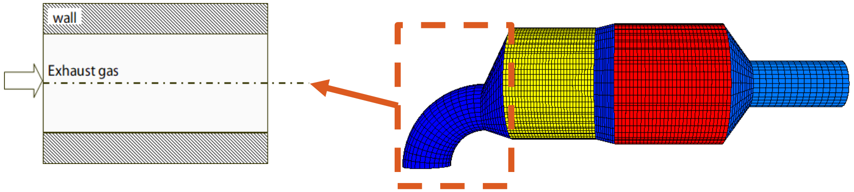


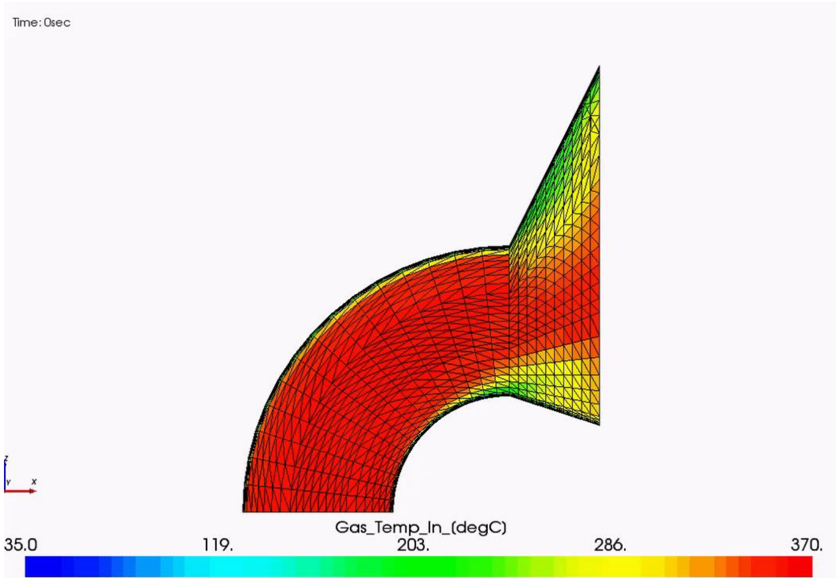
Dual wall with airgap

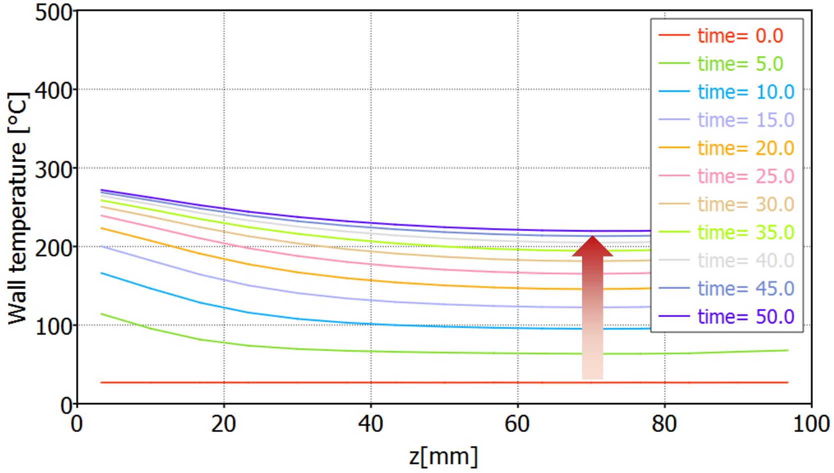
Transient wall temperature effect

Initial wall temperature = 27°C
Constant inlet temperature = 350°C

Single wall inlet pipe

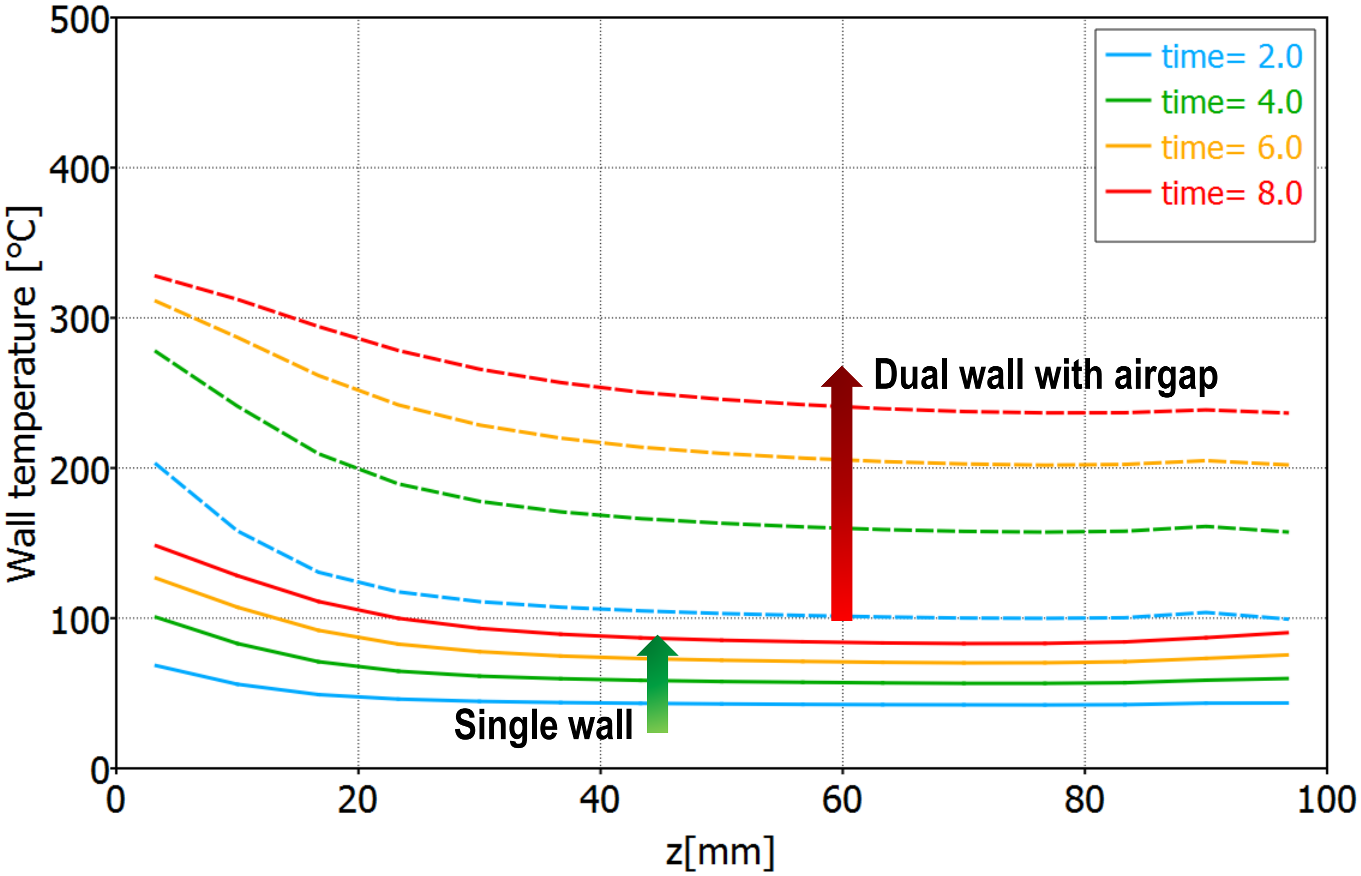


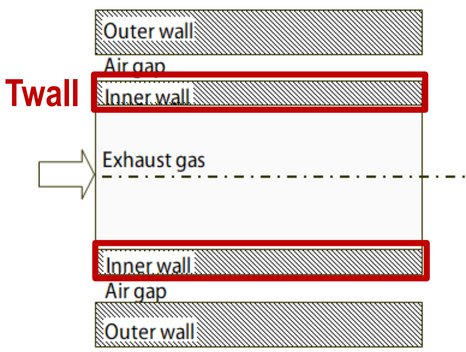


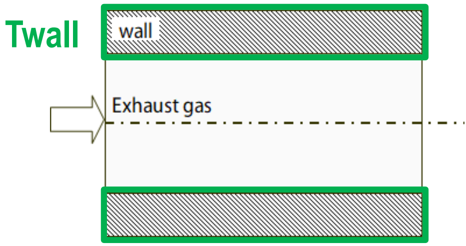


- Slow wall heat-up due to its thermal mass
- Wall temperature affects the inlet gas temperature profile

Single wall v.s. airgap configuration

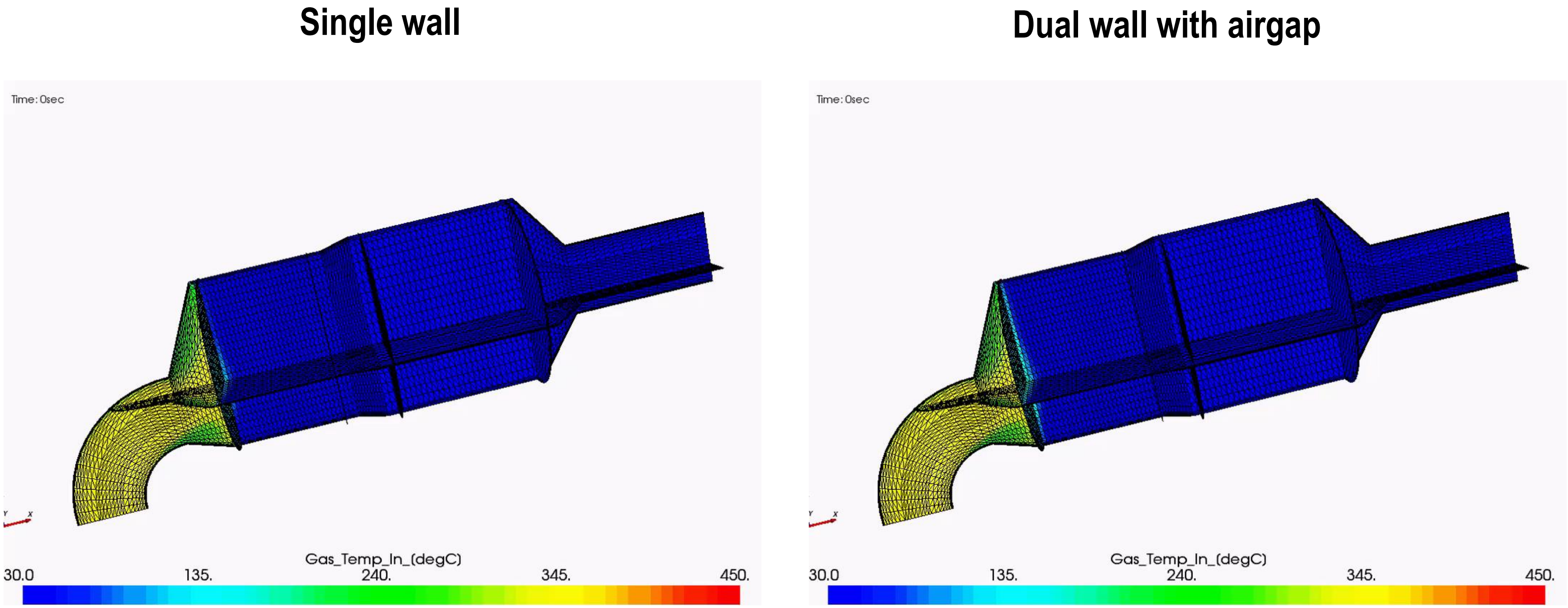



Dual wall with airgap


Single wall pipe

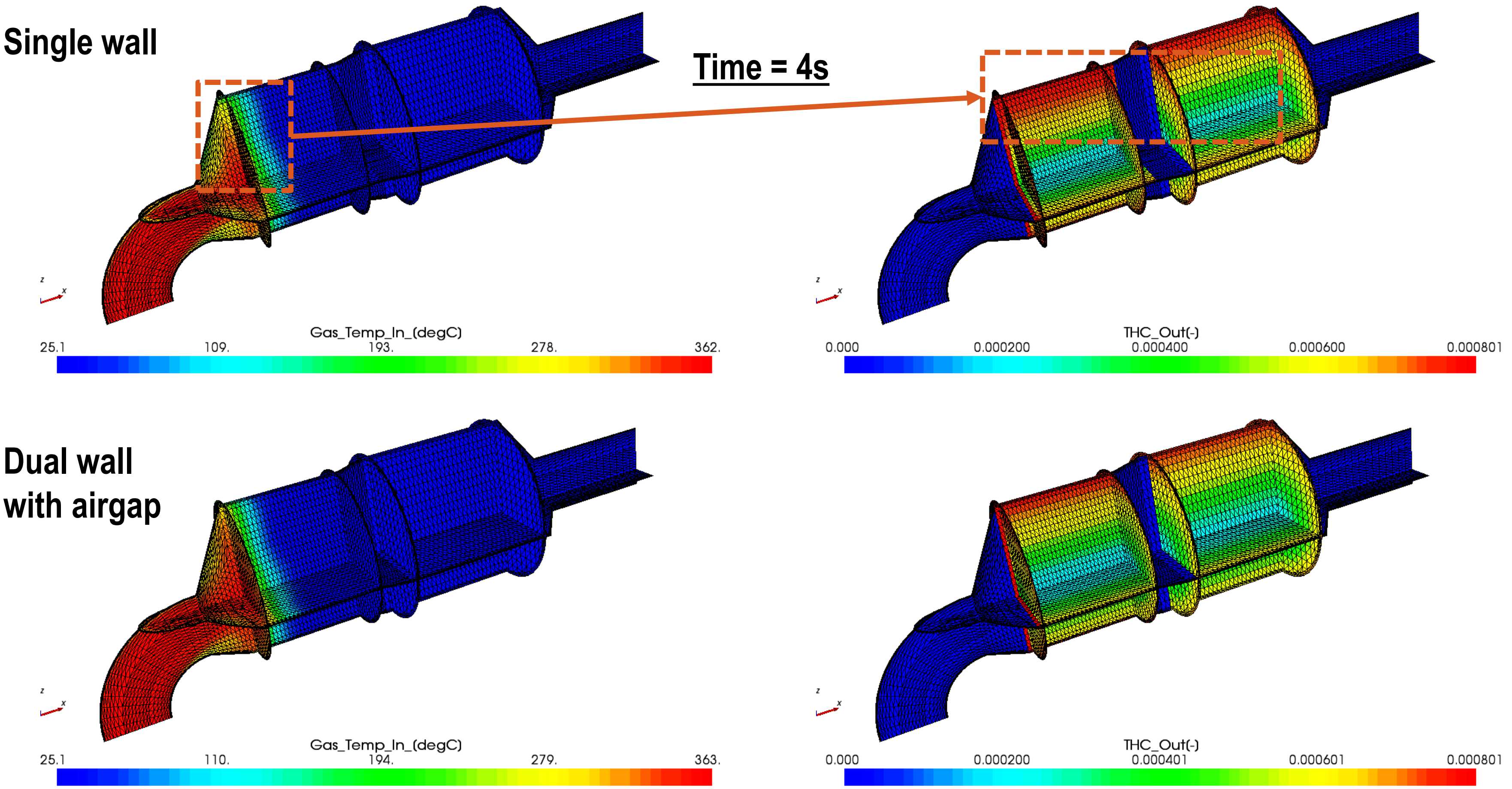
- Single wall configuration has lower wall temperatures due to higher heat losses
- Low thermal mass results in higher temperatures for the airgap configuration

Inlet temperature distribution



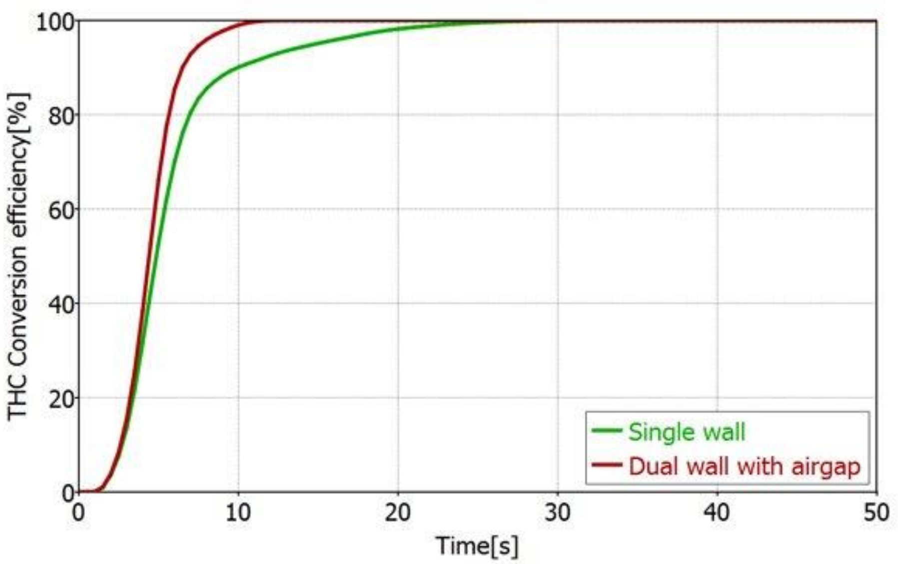
- Gas temperature at the periphery for the single wall configuration is lower compared to airgap configuration
- Such non-uniformities can affect the performance of the catalyst locally.

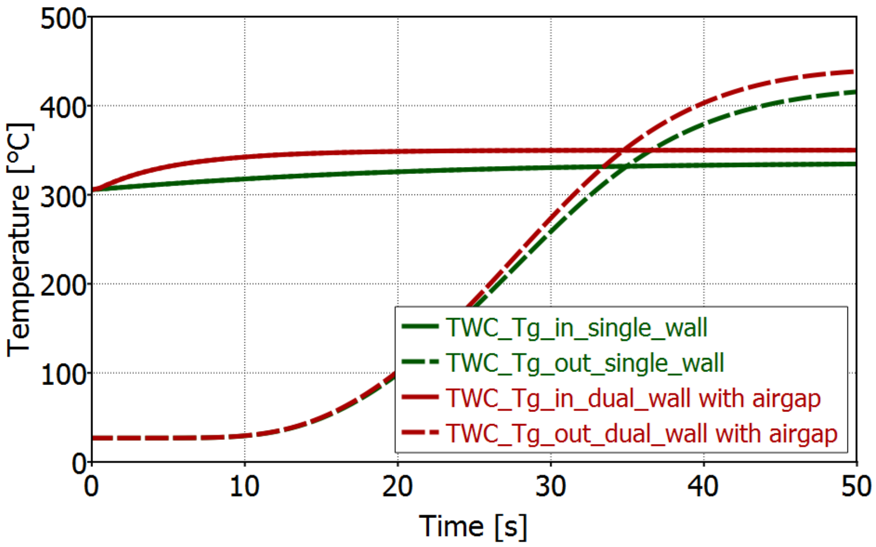
Effect of temperature non-uniformity to THC emissions



- Lower gas temperatures at the periphery reduces THC conversion at this area.
- Higher THC concentration for the single wall configuration.

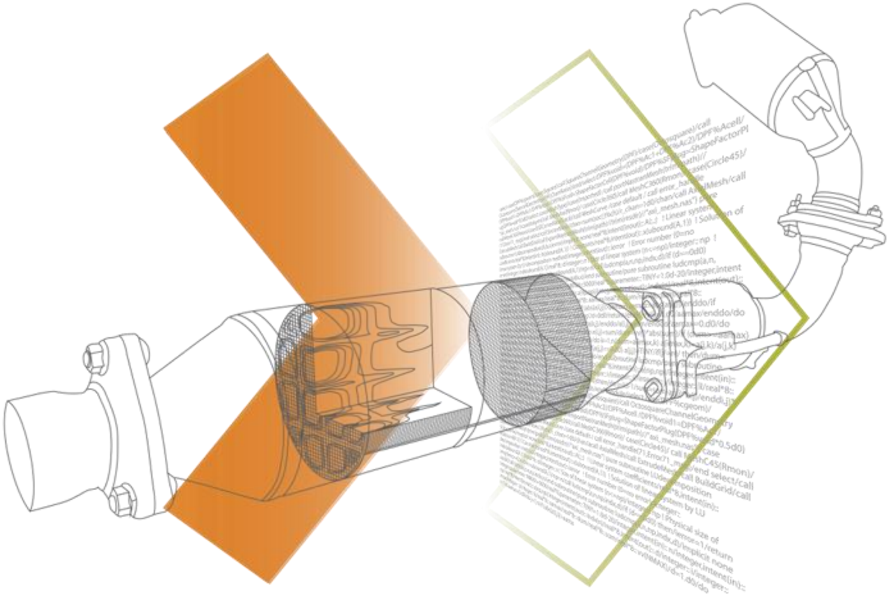
THC emissions





- Faster THC conversion efficiency for airgap compared to single wall configuration.
- This effect is due to different gas temperature non-uniformities at the TWC entrance

exothermia
EFFICIENCY. PREDICTED.



Drop to idle

Drop to idle issue

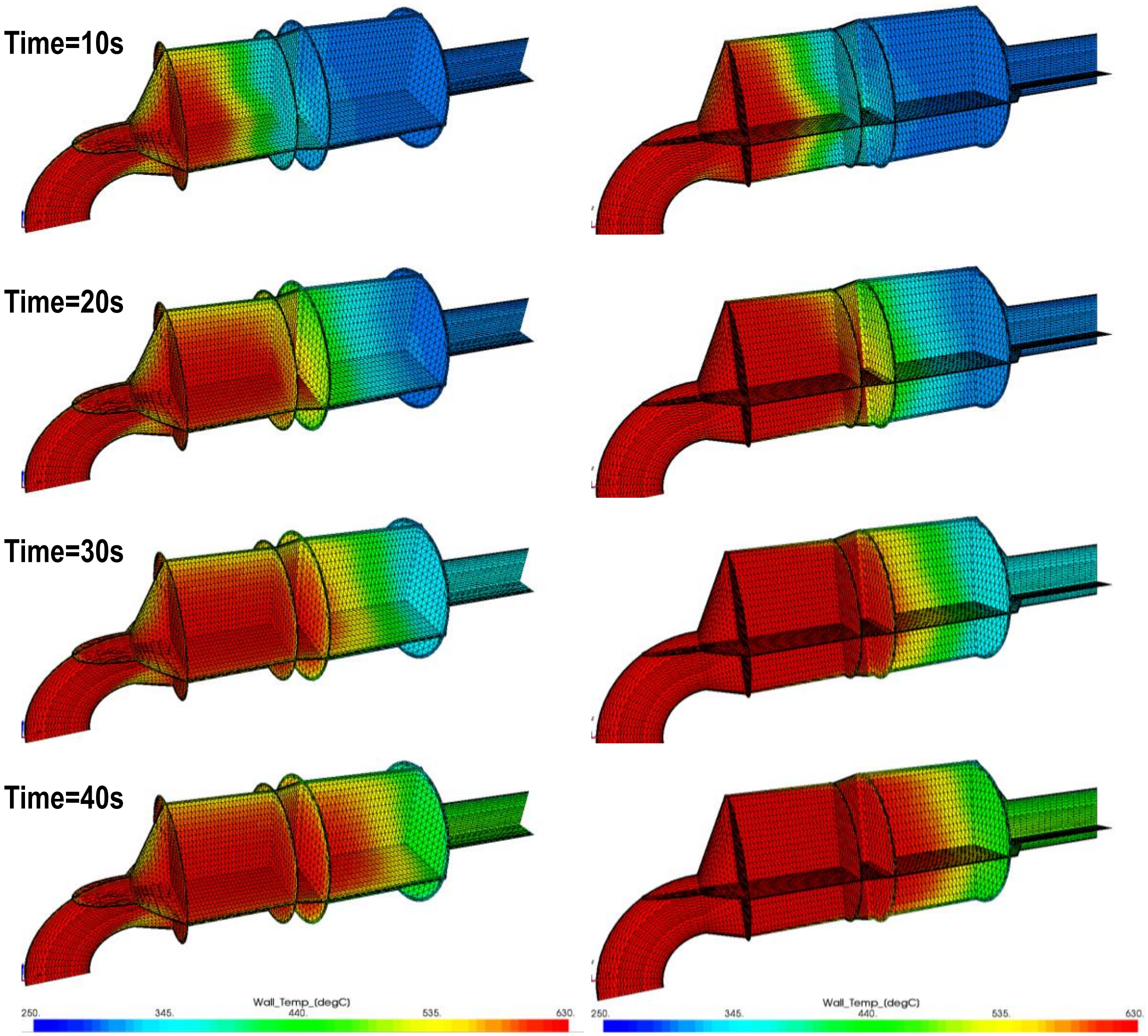
Drop to idle: The increase in oxygen concentration and the decrease in exhaust flow rate resulting in uncontrolled filter regeneration.

- The particulate matter (PM) emitted be the gasoline engine is collected and then burned in Gasoline Particulate Filter (GPF).
- The impact of the inlet cone on the GPF behavior is investigated.
- Initial GPF soot loading 2.9 g/l

Inlet scenario	0 – 60 s	60 – 90 s
Inlet temperature [°C]	600	600-350
Mass flow rate [kg/s]	$2.5e^{-2}$	$5e^{-3}$
Species concentration		
CO [%]	0.75	0.0
O2 [%]	0.0	20
CO2 [%]	10	0.0
H2O [%]	7.5	0.0
H2 [%]	0.25	0.0
NO [ppm]	650	0.0
C3H6 [ppm]	800	0.0

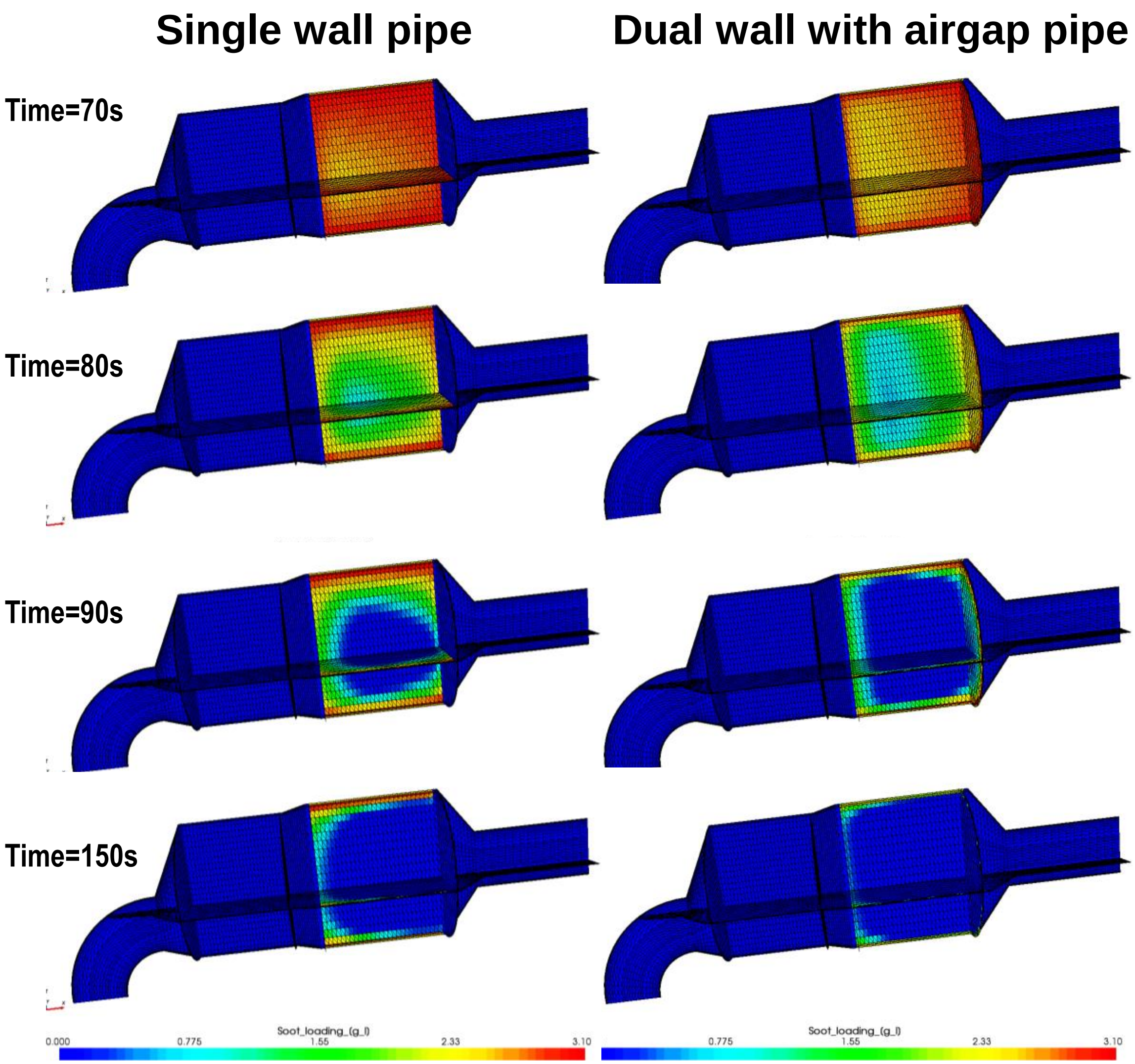
Warm-up - Effect of inlet pipe insulation to wall temperature

Single wall pipe **Dual wall with airgap pipe**

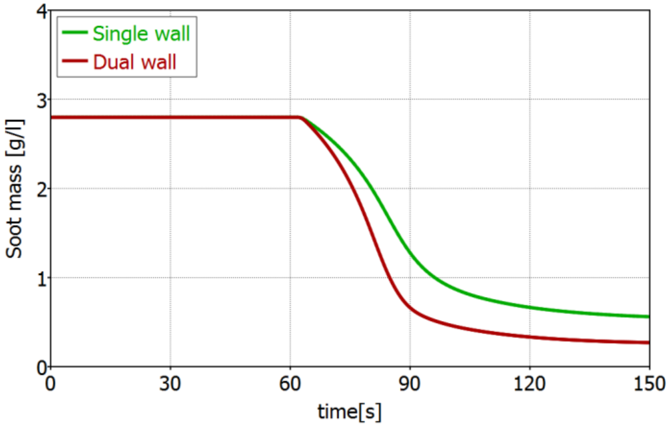


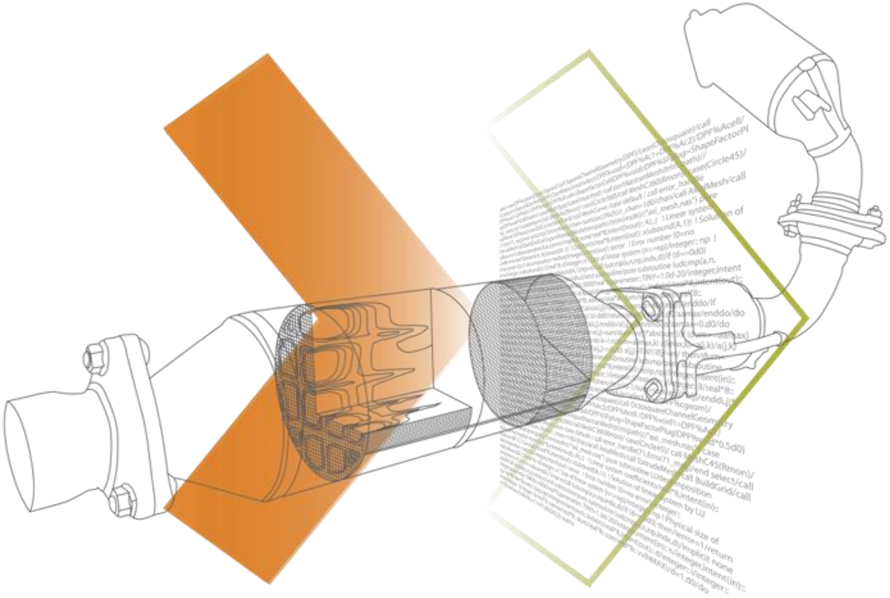
- Wall temperature in dual wall is more **uniform** compare to single wall inlet pipe configuration during warm-up period.
- For single wall pipes, the temperature at the periphery of both inlet pipes and monoliths show high discrepancy due to the heat losses.

DTI - Effect of temperature to soot distribution



- The non-uniform temperatures in the filter result in non-uniform soot distribution during the regeneration.
- At the end of the drop-to-idle event the dual wall configuration has regenerated more soot than the single wall.

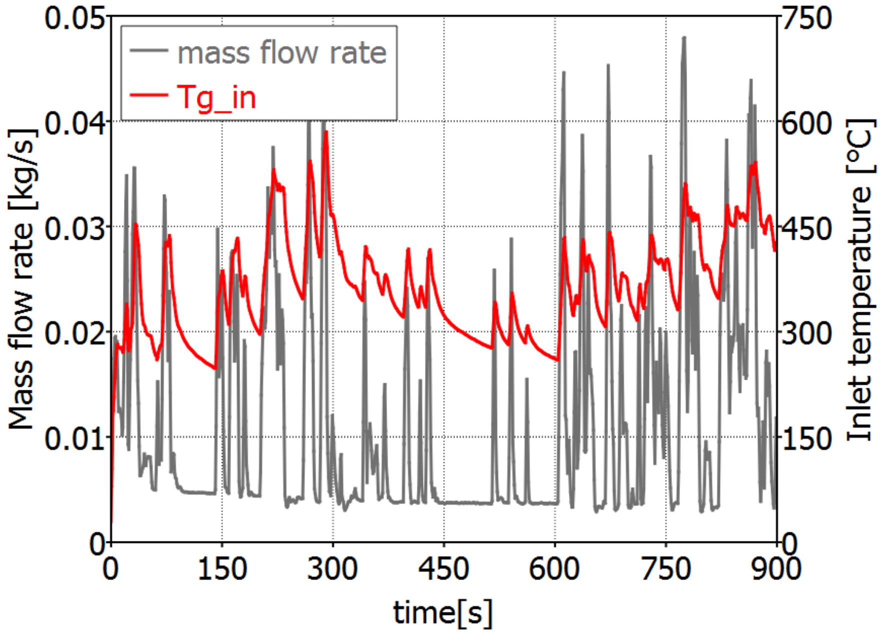


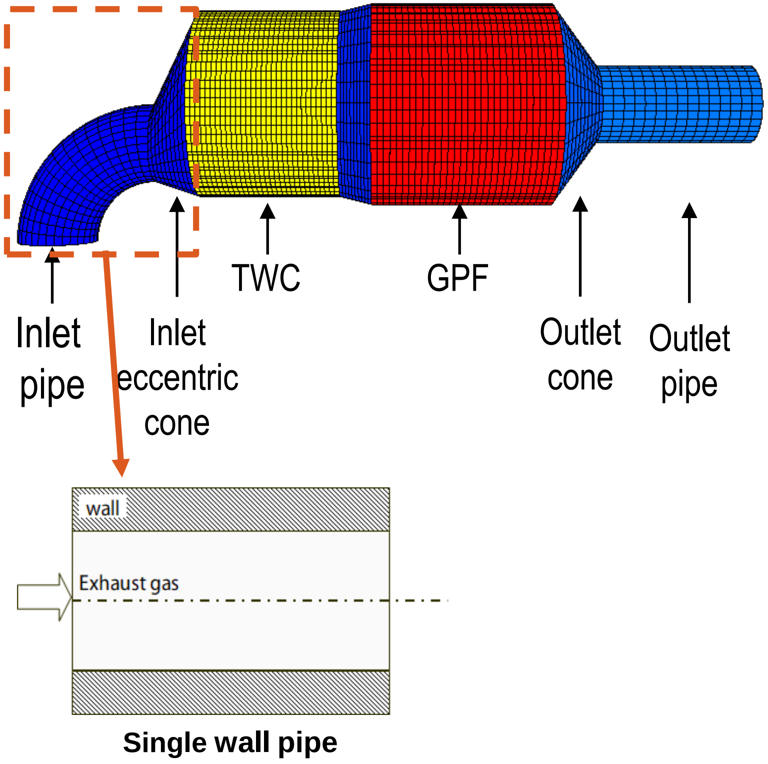


WLTC

Problem statement

- **Problem description**: Investigate the effect of 3D simulation on conversion efficiency of the species during WLTC. A single wall inlet pipe is simulated.
  - Case1: 1D
  - Case 2: 3D/OpenFoam

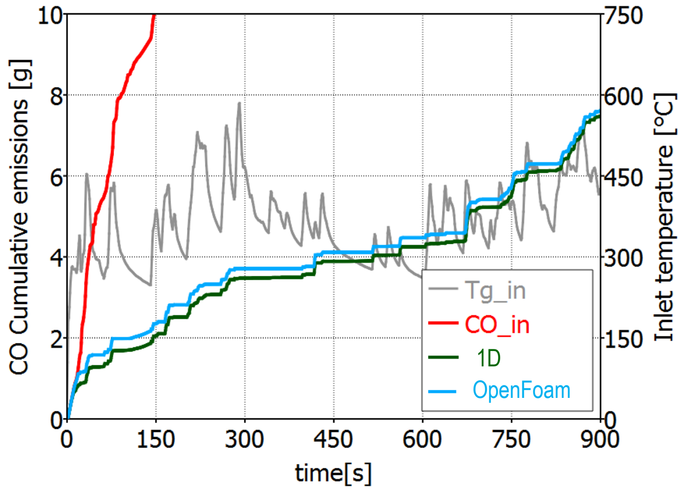




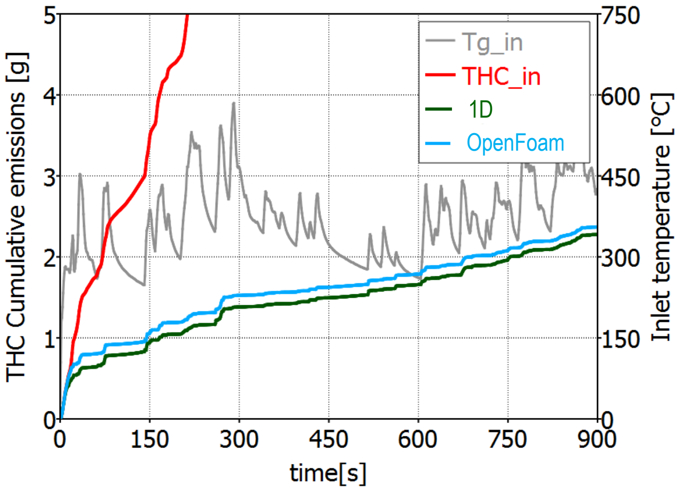
Single wall pipe

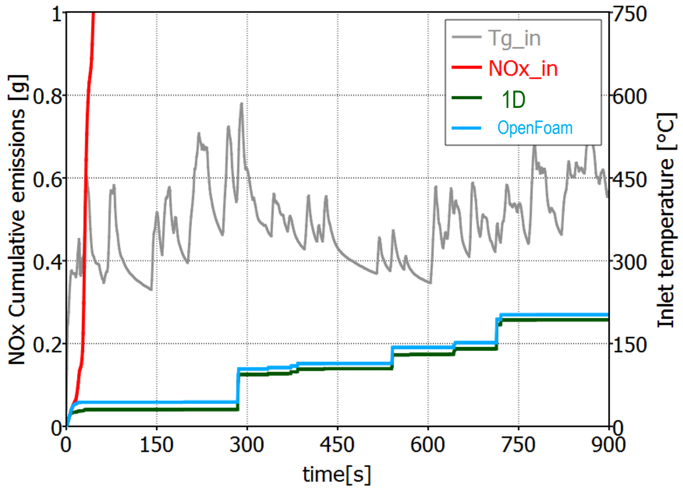
WLTC – Cumulative emissions

exothermia
EFFICIENCY. PREDICTED.



1D





- Flow, temperature and species **non-uniformities** inside the monolith affect the reactivity of the species, resulting in differences in cumulative conversion efficiency.
- Approximately CPU time 2 days in a usual PC

Conclusions

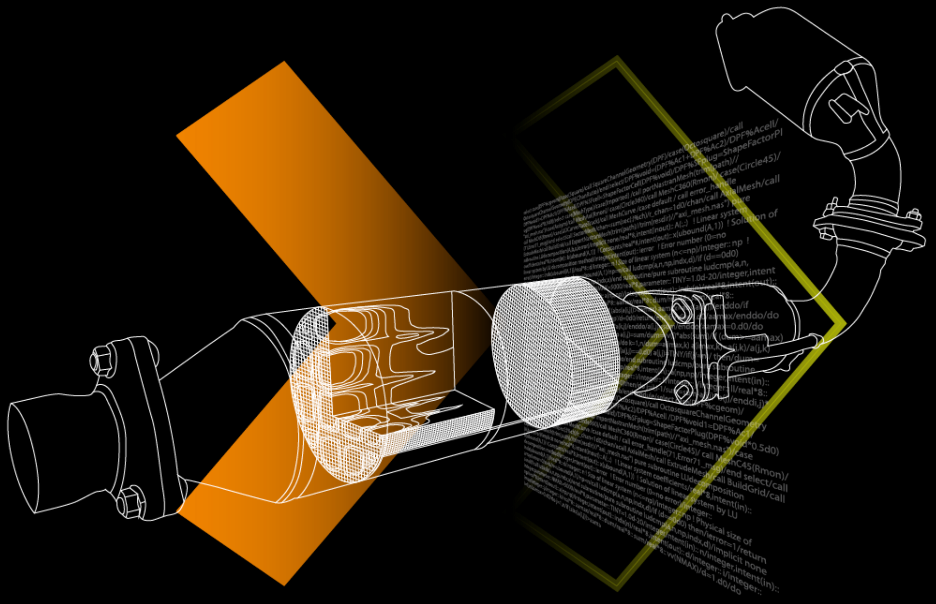
A fully integrated OpenFOAM/Exothermia suite approach is presented able to predict the effect of **flow uniformity** and **wall configuration** on exhaust system performance.

The main advantages of the proposed approach are:

- Detailed solution of the upstream and downstream geometry
- Detailed chemistry and filtration models
- Detailed heat/mass transfer models
- Multiple monolith components
- Metal parts thermal response calculated to provide proper time dependent boundary condition
- Parallel simulations
- Easy setup and post-processing
- Transient driving cycles are solved within days on normal PC

exothermia

EFFICIENCY. PREDICTED.



Thank you for your attention!