Integrating Filtration Mechanism with a 3D Diesel Particulate Filter (DPF) Model using STAR-CCM+

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Objective

- To study quantitative analysis of soot filtration processes in DPF (diesel particulate filter) systems by developing a three dimensional model using a commercial CFD package, STAR-CCM+.

- To analyze the time evolution and spatial distributions of local filtration parameters – e.g. porosity, soot mass, collection efficiency, soot cake profile - for each filtration period, along with evaluations of flow properties and pressure drop characteristics across the DPF.
Background (1/2)

Diesel Engine

Pros: High Thermal Efficiency, Fuel Economy, Torque, Low Emission (CO, UHC)
Cons: Noise, Vibration, $, Emission (PM, NOx)

PM and NOx are the major emissions regulated. (USA: EPA Tier 4, EU: Euro 5 / 6)

- NOx reduction by SCR and/or EGR
- PM needs to be reduced in both mass and number... Arising issue for GDI engines, too!

Diesel Particulate Filter (DPF)

- Highway diesel vehicles are required to meet the stringent PM emission standards.
- Physically trap (Filtration), and chemically oxidize PM (Regeneration) periodically.
- Uncontrolled regeneration may occur which causes system failure due to highly exothermic reaction.

Prediction of particulate deposition in the porous filter wall is important.
Background (2/2)

- Two Approaches in Filtration Modeling
  - **Lagrangian**: Qualitative analysis by tracking particle trajectories with appropriate B.C.s.
  - **Eulerian**: Quantitative analysis of soot filtration process by coupling specific filtration algorithms.


**Theoretical Analysis (1/2)**

### Pressure Drop Model

\[
\Delta P = \Delta P_{\text{porous wall}} + \Delta P_{\text{soot cake}} + \Delta P_{\text{friction}} + \Delta P_{\text{cont/expans}}
\]

\[
= \left( \frac{\mu}{k_0} u_w w_s + \beta \rho u_w^2 w_s \right) + \left( \frac{\mu}{k_{\text{soot}}} \int_0^w u(x) \, dx \right) + \left( \frac{\mu F}{3a^2} U_{o,\text{in}} L \xi + \frac{\mu F}{3a^2} U_{o,\text{out}} L \xi \right) + \left( \frac{\zeta_{\text{cont}}}{2} + \frac{\zeta_{\text{exp}}}{2} \right)
\]

**Darcy-Forchheimer's Law**

- Each velocity term is defined as,

\[
\begin{align*}
\mathbf{u}_w &= \frac{Q_o}{A_{\text{filt}}} = \frac{U_o A_o}{4aL} = \frac{U_o a^2}{4aL} = \frac{U_o a}{4L} \\
\int_0^w u(x) \, dx &= \int_0^w \frac{Q_o}{A_{\text{filt}}(x)} \, dx = \int_0^w \frac{Q_o}{4(a - 2(w - x))L} \, dx = \frac{Q_o}{8L} \ln \left( \frac{a}{a - 2w} \right) \\
U_{o,\text{in}} &= \frac{Q}{\sum_{\text{inlet}} A_o} = \frac{\pi D^2}{4} \frac{1}{2} \frac{1}{2} \frac{(a - 2w)^2}{(a + w_s)^2} = \frac{\pi D^2 \sigma (a - 2w)^2}{16Q} \\
Q_o &= \frac{Q A_o}{\sum_{\text{inlet}} A_o} = \frac{Q(a - 2w)^2}{\pi D^2} \frac{1}{2} \frac{1}{2} \frac{(a - 2w)^2}{(a + w_s)^2} = \frac{16Q(a + w_s)^2}{\pi D^2} \\
u &= \frac{Q}{Na^2}
\end{align*}
\]

- Clean filter condition for \( A_o \)
- Soot cake thickness \((w)\) for \( A_o \)

Half-cut sample for experiment
Theoretical Analysis (2/2)

Soot Filtration Model

- Unit Collector Mechanism
  - Clean unit cell
  - Partially loaded unit cell
  - Completely loaded unit cell

\[ d_{c0} = \frac{3(1 - \varepsilon_0)}{2\varepsilon_0} d_{pore} \]

\[ d_{c0}^3 \frac{3}{b^3} = 1 - \varepsilon_0 \]

\[ \varepsilon(i, t) = 1 - \left( \frac{d_c(i, t)}{d_{c0}} \right)^3 (1 - \varepsilon_0) \]

\[ d_c(i, t) = 2 \left( \frac{3}{4\pi} \frac{m_{local}(i, t)}{\rho_{soot,wall}} + \left( \frac{d_{c0}}{2} \right)^3 \right)^{\frac{1}{3}} \]

\[ k(i, t) = k_0 \left( \frac{d_c(i, t)}{d_{c0}} \right)^2 f(\varepsilon(i, t)) \frac{f(\varepsilon)}{f(\varepsilon_0)} \]

\[ \phi(t) = \frac{(d_c(i, t))^2 - d_{c0}^2}{(\Psi b)^2 - d_{c0}^2} \]

Key parameters for CFD code (UDF) to specify region properties

Collection Efficiency

- Diffusional Deposition (\( \eta_D \))

- Flow-line Interception (\( \eta_R \))

\[ \eta_D = 3.5 \ g(\varepsilon) \ Pe^{-\frac{2}{3}} = 3.5 \ g(\varepsilon) \left( \frac{U_i d_c}{D} \right)^{-\frac{2}{3}} \]

\[ \eta_R = 1.5 \ N_R^2 \ \frac{\left( g(\varepsilon) \right)^3}{(1 + N_R)^{\frac{3-2\varepsilon}{3\varepsilon}}} \]

\[ \eta_{DR} = \eta_D + \eta_R - \eta_D \eta_R \]

\[ E(i, t) = 1 - \exp \left( -\frac{3\eta_{DR} (1 - \varepsilon(i, t)) \Delta y}{2\varepsilon(i, t) d_c(i, t)} \right) \]

Key parameters for User Code to obtain local soot mass (\( m_w \))
Experiment

2” x 6” cordierite DPF Test Results

Clean Filter Test

- Clean filter permeability ($k_o$) and particle-laden flow properties are directly measured.
- Soot cake permeability ($k_{s,cake}$), particle density ($\rho_s$), and soot cake porosity ($\epsilon_{s,cake}$) can be estimated.
- Packing densities ($\rho_{s,wall}$, $\rho_{s,cake}$) are assumed.

Soot Loading Test

- Pressure drop vs. time for low flow rate (7.4 SCFM) and high flow rate (9.0 SCFM).
- Pressure drop vs. volume flow rate for 100 CPSI ($w_s=17$ mils) and 200 CPSI ($w_s=12$ mils).

PM Mass Concentration and PM Size Distribution

TEOM and SMPS measurements for different flow rates.
Model Setup (1/2)

- **Domain Setup**
  - Geometry is based on a 200CPSI, lab-scaled (2”x 6”) cordierite filter with regions of upstream flow and soot cake formation.

- **Meshing**
  - Volume meshes are generated by using **Trimmer** for porous regions (filter wall, soot cake), and **Polyhedral** for fluid and solid regions (channels, plugs).

### Domain Setup
- Trimmer is exclusively used for filter wall, consisting of 10 separate porous regions, to represent soot filtration. (Growth rate = 1, Cell size = thickness of each region)

### Meshing
- Total 2,013,762 cells
  - All cells in wall regions are regular hexahedrons

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**POROUS REGION**
- Filter wall
- Soot cake

**FLUID REGION**
- Upstream
- I/O Channels

**SOLID REGION**
- Plugs

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*Integrating Filtration Mechanism with a 3D Diesel Particulate Filter (DPF) Model using STAR-CCM+*
Model Setup (2/2)

Physical Assumptions
1. Fluid: 3D, Ideal gas, Laminar, Incompressible
2. Implicit unsteady method (2\textsuperscript{nd} order temporal discretization, $\Delta t = 0.05$ sec)
3. Segregated flow & energy solver (2\textsuperscript{nd} order convection scheme, $URF=0.5P$, $0.2V$)
4. Convective heat loss
5. No flow in the axial(z) direction in wall regions
6. Homogeneous distribution of particulates in the flow
7. Particle properties ($d_p=54.5$ [nm], $\rho_p=2.87$ [g/cm\textsuperscript{3}]) evaluated by experiments

Boundary Conditions

- **Mass flow Inlet**: $3.05E-6$ [kg/s] (= 7.4 SCFM)
- **Pressure Outlet**: 125.44 [kPa] (= 18.2 psi)
- **Slip**: Define geometrically symmetry planes/surfaces
- **Adiabatic**: Neglect heat loss for thermal condition at channel inlet
- **Convection**: Specify convection flux across the boundary to environment (ambient)

\[
\bar{h}_{conv} = \frac{Q}{A_{eq}\Delta T} = \frac{\dot{m}c_p(T_i - T_o)}{A_{eq}(T - T_{amb})}
\]
\[
R_{t,f} = \frac{1}{\kappa} w_r
\]

Potential energy
Chemical reactions
Compression effect
Expansion effect
Plugging effect
Soot Cake Transport
Ash formation
Filtration Algorithm (1/3)

- Cell Value Localization

  \[ m_{in}(t) = \chi_s Q_s \Delta t \]

  \[ 0 \leq \text{Soot Cake Mass Fraction} \leq 1 \]

  **Problem**

  : To make each CFD cell acting as a unit collector, cell index must be ordered, so that the cell values can be transferred in certain direction.

  Structured meshing is NOT allowed in standard CFD tools

  **Solution**

  : Having the same cell indices in \( y \) direction by meshing each wall layers, separately.
**Filtration Algorithm (2/3)**

### Built-in Function Utilization

**Problem**

- Classic unit collector mechanism causes a **circulation** error during initialization. Thus, Eq.(3) needs to be modified to account $E(i, t - 1)$.

$$\begin{align*}
\varepsilon(i, t) &= 1 - \left(\frac{d_c(i, t)}{d_{c0}}\right)^3 (1 - \varepsilon_0) \quad \ldots \text{Eq. (1)} \\
d_c(i, t) &= 2 \left(\frac{3}{4\pi} \frac{m_{\text{local}}(i, t)}{\rho_{\text{soot,wall}}} + \left(\frac{d_{c0}}{2}\right)^3\right)^{1/3} \quad \ldots \text{Eq. (2)} \\
m_{\text{local}}(i, t) &= m_{\text{in}}(i, t) E(i, t) \quad \ldots \text{Eq. (3)} \\
E(i, t) &= 1 - \exp\left(-\frac{3\eta_{DR} (1 - \varepsilon(i, t)) \Delta y}{2\varepsilon(i, t) d_c(i, t)}\right) \quad \ldots \text{Eq. (4)}
\end{align*}$$

...but, time array can **NOT** be handled through UDFs.

**Solution**

- **Store** current ($t$) cell values using **Table** function, then **access** the data by interpolating the table as fields (UDF) at the next time step ($t+1$).

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**Recall**

- $\varepsilon(i, t) = 1 - \left(\frac{d_c(i, t)}{d_{c0}}\right)^3 (1 - \varepsilon_0)$
- $d_c(i, t) = 2 \left(\frac{3}{4\pi} \frac{m_{\text{local}}(i, t)}{\rho_{\text{soot,wall}}} + \left(\frac{d_{c0}}{2}\right)^3\right)^{1/3}$
- $m_{\text{local}}(i, t) = m_{\text{in}}(i, t) E(i, t)$
- $E(i, t) = 1 - \exp\left(-\frac{3\eta_{DR} (1 - \varepsilon(i, t)) \Delta y}{2\varepsilon(i, t) d_c(i, t)}\right)$
Filtration Algorithm (3/3)

- Recursive Operation

\[ m_{in} = \chi_s Q_s \Delta t \]

- Problem

- Flow changes with engine operating condition.
  \[ \rightarrow \text{Local soot mass must be accumulated through time integral, considering collection efficiency.} \]

...but standard CFD code do NOT have ability to allow mathematical recursiveness through UDFs.

- Solution

- Couple User Code and Monitor function.
Computing Environment

- Argonne TRACC (*Transportation Research and Analysis Computing Center*)
  - A national user facility to meet US DOT advanced computation needs.
  - A focal point for computational research for transportation applications.
  - Linked to federal and non-federal R&D facilities, regional, state and city departments of transportation, and university research centers.

- High Performance Clusters
  - Total 3,968 cores in 220 compute nodes
    - **Zephyr**: 16 AMD 6273 (cores/CPU) * 2 (CPUs/node) * 92 (nodes)
    - **Phoenix**: 4 AMD 2378 (cores/CPU) * 2 (CPUs/node) * 128 (nodes)

*10 Iterations Benchmark Test*

- 1 core: Local (3.4GHz, 16GB)
- 2 cores: Local
- 4 cores: Local
- 8 cores: Cluster (2.3GHz, 32GB)
- 16 cores: Cluster

**Total solver elapsed time [s]**

- Iteration [#]
- 1 2 3 4 5 6 7 8 9 10

**Summary**

- **Objective**
- **Background**
- **Theoretical Analysis**
- **Experiment**
- **Model Setup**
- **Filtration Algorithm**
- **Computing Environment**
- **Model Results**
- **Future Work**
- **Acknowledgement**

**Integrating Filtration Mechanism with a 3D Diesel Particulate Filter (DPF) Model using STAR-CCM+**
Model Results (1/5)

- Channel-flow Profiles
  - Pressure
    - [KPa]
    - 300s
    - 600s
    - 1000s
  - Velocity
    - [m/s]

- Pressure Drop Characteristics
  - Effect of percolation factor (ψ)
    - Soot Loading [g/L]
    - Depth filtration
    - Transition
    - Cake filtration
    - Experiment
    - Model (ψ=0.9)
    - Model (ψ=0.86)
Model Results (2/5)

Wall-flow Rearrangements

- Pre-transition regime
- Post-transition regime

<table>
<thead>
<tr>
<th>Wall-flow</th>
<th>[m/s]</th>
<th>Normalized Channel Length [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wall-through Velocity</td>
<td>0.020</td>
<td>0.028</td>
</tr>
<tr>
<td>Depth filtration</td>
<td>30s</td>
<td>90s</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Normalized Channel Length [-]</th>
<th>30s</th>
<th>90s</th>
<th>120s</th>
<th>300s</th>
<th>600s</th>
<th>1000s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Velocity Avg.</td>
<td>1.0E-03</td>
<td>2.0E-03</td>
<td>3.0E-03</td>
<td>4.0E-03</td>
<td>3.0E-03</td>
<td>2.0E-03</td>
</tr>
<tr>
<td>Std. Deviation</td>
<td>UNIFORMIZED</td>
<td>ACCELERATED</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Model Results (3/5)

- Local Soot Mass Deposited
  - \( y-z \) plane \((@ x = 1/4a)\)
  - \( x-y \) plane \((@ z = 1/2L)\)

- Deposited soot profiles

Integrating Filtration Mechanism with a 3D Diesel Particulate Filter (DPF) Model using STAR-CCM+
Model Results (4/5)

- **Local Collection Efficiency** ($d_p=54.5$ nm)
  - y-z plane (@ $x = 1/4a$)
  - x-y plane (@ $z = 1/2L$)
Model Results (5/5)

- Soot Cake Layer Properties
  - Porosity ($\rho_{s,cake}=120 \, \text{kg/m}^3$)
  - Thickness (@ 1000 s)

Maintain 0.99↑ during first 1000 seconds of filtration
A 3D CFD model was successfully developed for quantitative analysis of transient soot filtration processes in a wall-flow type DPF.

The local value and rearrangement behaviors of each filtration parameter are well predicted within isotropically discretized meshes in the multi-layered porous wall regions.

Self-developed user subroutines, developed on basis of the unit collector mechanism, are integrated with the CFD code.

Built-in functions – Table, Monitor, UDF – were combined and fully coupled with algorithm to calculate the local value of soot mass and collection efficiency in the wall layer at each time step.

Results were visually demonstrated at the channel length scale in 3D, representing correlations among wall flow pattern, soot mass distribution, and soot cake profile.
Future Work

- Modeling additional porous and fluid regions
  - Create additional soot cake regions near the surface of the plugs to take into account plugging effects.
  - Create the downstream region to consider flow-expansion effects.

- Integrating PM oxidation reaction mechanisms
  - Utilize soot filtration simulation results (soot mass distribution and soot cake profile) for the initial state of regeneration simulation.
  - Apply chemical kinetics of soot oxidation in consideration of the effects of O₂, CO, NO₂ and HCs (additional user subroutines need to be developed).
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