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Simulating Catalytic Reaction and Soot Oxidation in Coated Particulate Filters: A Simplified Modelling Framework Including Diffusion Effects

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Concept

- Simplified framework for simulating reaction in coated particulate filters
 - Avoids discretisation in the through wall direction

- In this presentation:
 - Will focus on the modelling approach, as that is what is new
 - Less on model predictions, as that is more well known
 - Except to demonstrate that the model gives plausible predictions

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Outline

- 01** Concept

- 02** Model description

- 03** Simulation conditions and parameters

- 04** Example simulations: Oxidation of gaseous components

- 05** Example simulations: Soot oxidation

- 06** Summary / Conclusions

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Included Diffusion Pathways

- 1) Diffusion between gas in channels and adjacent walls
 - Similar to flow-through monoliths

- 2) Diffusion between inlet and outlet channels along path of convective flow from inlet channel to outlet channel
 - Analogous to axial dispersion in a packed bed reactor
 - Imagine filter wall as being like a packed bed reactor

- 3) Diffusion between gas passing through filter wall and catalyst phase
 - Analogous to external transport in a packed bed
 - Not included in most particulate filter models
 - Enables a simplification in this model

Model Structure: Soot & Ash Cakes, Filter Wall

- Filter discretised axially
- For each axial element, divide cake and wall into layers
 - Soot cake, ash cake, filter wall
 - Can vary thickness of each layer
 - Wall split into two layers
 - One catalysed, one inert
 - In either order
 - Allows through-wall position of catalyst to be varied
- Transport by:
 - Convection from inlet channel to outlet
 - Diffusion between channels along same path

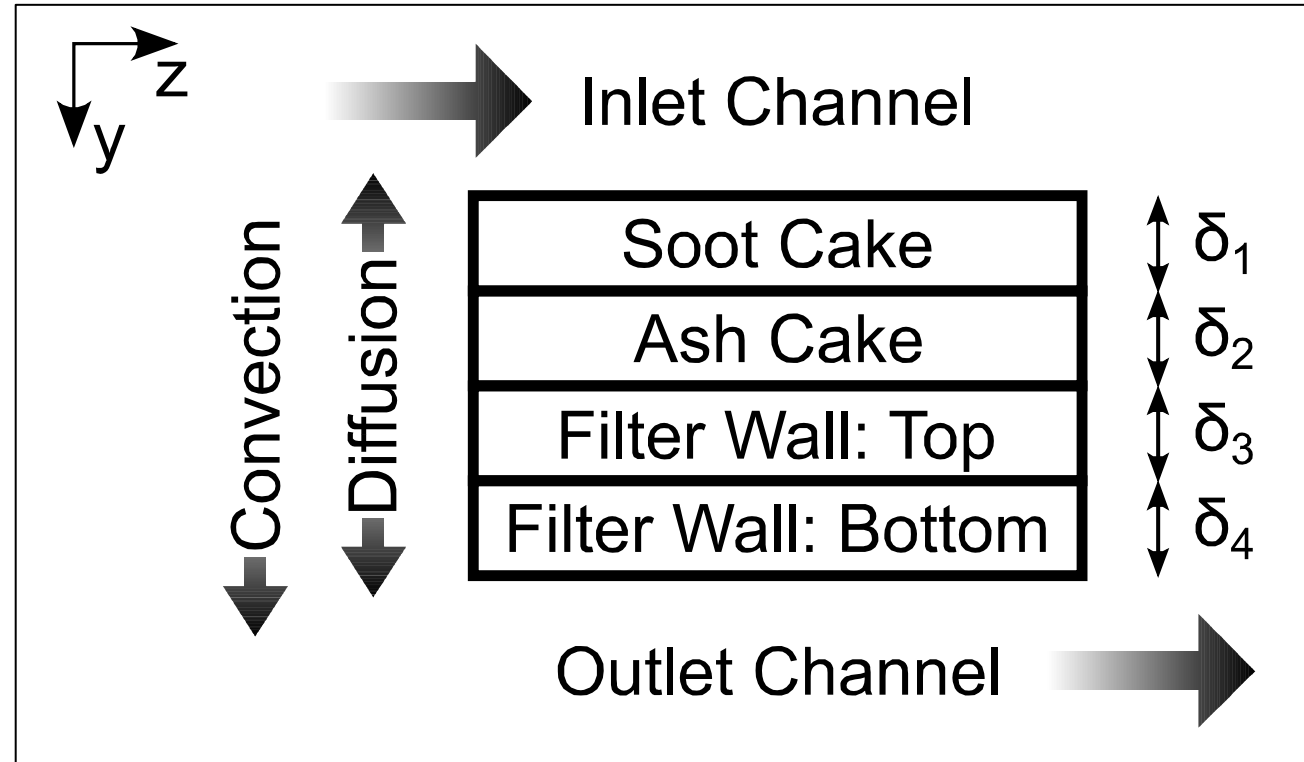
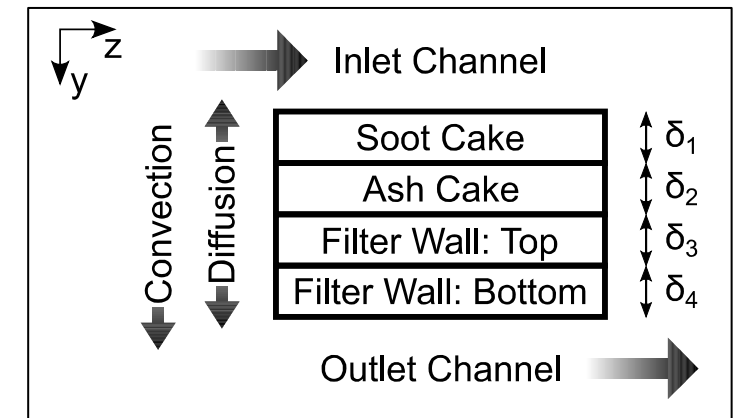


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Simplifications

- Simplifications:
 - Discretise filter axially
 - Assume all layers are slabs/cuboids – neglect taper on soot and ash cakes
 - Soot oxidation is first order in NO_2 and O_2
 - Use single, representative concentration for each species in the catalyst phase in each axial element
 - Probably, most significant approximation
- Consequences (benefits):
 - Component mass balance for each layer is a second-order, linear differential equation
 - These have an analytical solution for the concentration of the species through the layer
 - Result in a system of linear simultaneous equations, which are easily solved (with linear algebra)



Component Mass Balances for Gas in Inlet and Outlet Channel

Differential equations

- Balance equations for inlet and outlet channels:

$$0 = -\frac{1}{M} \frac{\partial d_i^2 \phi_i x_{gi,j}}{\partial z} + p_i k_{mi,j} (C_{gw0,j} - x_{gi,j} C_{Ti}) - \frac{4\psi_w C_{gw0,j}}{\rho_{gw}} \quad \text{Inlet channel}$$

$$0 = -\frac{1}{M} \frac{\partial d_o^2 \phi_o x_{go,j}}{\partial z} + p_o k_{mo,j} (C_{gwm,j} - x_{go,j} C_{To}) + \frac{4\psi_w C_{gwm,j}}{\rho_{gw}} \quad \text{Outlet channel}$$

Convection along channel Diffusion to channel wall Convection to/from wall

d_i, d_o	=width of inlet/outlet channel	$x_{gi,j}, x_{go,j}$	=mole fraction in inlet/outlet channel
M	=molar mass of gas	z	=axial coordinate
$C_{gw0,j}$	=concentration of gas entering wall	ρ_{gw}	=density of gas in wall
$C_{gwm,j}$	=concentration of gas leaving wall	ϕ_i, ϕ_o	=mass flux along inlet/outlet channel
C_{Ti}, C_{To}	=total gas concentration in channel	ψ_w	=mass flow through one wall per unit length of filter
$k_{mi,j}, k_{mo,j}$	=mass transfer coefficients		
p_i, p_o	=channel perimeter		

Component Mass Balances for Gas in Inlet and Outlet Channel

Discretised equations

- Balance equations for inlet and outlet channels:

$$0 = -\frac{1}{M} \frac{\partial d_i^2 \phi_i x_{gi,j}}{\partial z} + p_i k_{mi,j} (C_{gw0,j} - x_{gi,j} C_{Ti}) - \frac{4\psi_w C_{gw0,j}}{\rho_{gw}}$$

$$0 = -\frac{1}{M} \frac{\partial d_o^2 \phi_o x_{go,j}}{\partial z} + p_o k_{mo,j} (C_{gwm,j} - x_{go,j} C_{To}) + \frac{4\psi_w C_{gwm,j}}{\rho_{gw}}$$

k = index of axial element
 $x_{gi,j,k}$ & $x_{go,j,k}$ = values at nodes
 $k_{mi,j,k}$ & $C_{gw0,j,k}$ = values in element centre
 δz = length of axial element

- These discretise to:

Use average of concentration at nodes before & after k^{th} axial element

- Inlet channel:

$$0 = \frac{d_{i,k-1}^2 \phi_{i,k-1} x_{gi,j,k-1}}{M} - \frac{d_{i,k}^2 \phi_{i,k} x_{gi,j,k}}{M} + p_i k_{mi,j,k} \left(C_{gw0,j,k} - \frac{[x_{gi,j,k-1} C_{Ti,k-1} + x_{gi,j,k} C_{Ti,k}]}{2} \right) \delta z - \frac{4\psi_{w,k} C_{gw0,j,k}}{\rho_{gw,k}} \delta z$$

- Outlet channel (except first element):

$$0 = \frac{d_o^2 \phi_{o,k-1} x_{go,j,k-1}}{M} - \frac{d_o^2 \phi_{o,k} x_{go,j,k}}{M} + p_o k_{mo,j,k} \left(C_{gwm,j,k} - \frac{[x_{go,j,k-1} C_{To,k-1} + x_{go,j,k} C_{To,k}]}{2} \right) \delta z + \frac{4\psi_{w,k} C_{gwm,j,k}}{\rho_{gw,k}} \delta z$$

- Outlet channel (first element):

$$0 = -\frac{d_o^2 \phi_{o,1} x_{go,j,1}}{M} + p_o k_{mo,j,1} (C_{gwm,j,1} - x_{go,j,1} C_{To,1}) \delta z + \frac{4\psi_{w,1} C_{gwm,j,1}}{\rho_{gw,1}} \delta z$$

Component Mass Balances Through Wall

General form

- In general, component mass balance for layer of wall has form:

$$\underbrace{D_{eT,j,k,l} \frac{\partial^2 C_{gw,j,k}}{\partial y^2}}_{\text{Diffusion}} - \underbrace{\frac{\phi_{w,k}}{\rho_{gw,k}} \frac{\partial C_{gw,j,k}}{\partial y}}_{\text{Convection}} + \text{source/sink terms} = 0$$

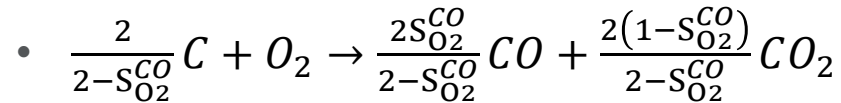
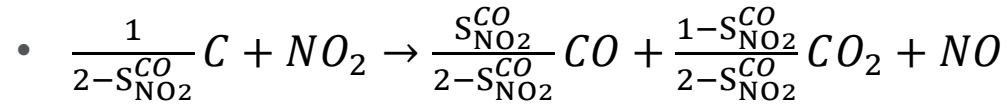
- $D_{eT,j}$ is effective diffusion coefficient for through-wall diffusion (subscripted T=through-wall)
 - This for diffusion along same path as convective flow through-wall
- Provided equation linear, this has solution of the form:
 - $C_{gw,j,k} = A_{j,k,l} e^{\alpha_{j,k,l} y} + B_{j,k,l} e^{\beta_{j,k,l} y} + \text{other terms}$
 - Create two arbitrary constants (A & B) per layer, per species, per axial element

$C_{gw,j,k}$	= Concentration in gas passing through wall	j	= index for species
y	= through-wall distance	k	= index for axial element
$\phi_{w,k}$	= mass flux through wall	l	= index for layer

Component Mass Balances Through Wall

Soot oxidation: Oxidants (NO₂ & O₂)

- Soot oxidises according to:



- Component mass balance for NO₂ in soot cake given by:

$$\bullet D_{eT,NO_2,k,1} \frac{\partial^2 C_{gw,NO_2,k}}{\partial y^2} - \frac{\phi_{w,k}}{\rho_{gw,k}} \frac{\partial C_{gw,NO_2,k}}{\partial y} - k_{NO_2,k} C_{gw,NO_2,k} = 0$$

- This has solution:

$$\bullet C_{gw,j,k} = A_{j,k,1} e^{\alpha''_{j,k,1} y} + B_{j,k,1} e^{\beta''_{j,k,1} y}$$

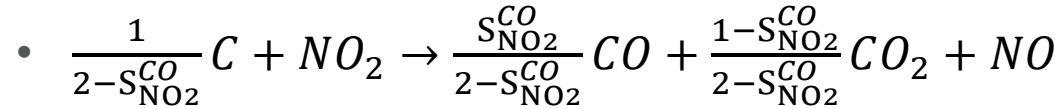
$$\bullet \text{where: } \alpha''_{j,k,1} = \frac{\phi_{w,k}/\rho_{gw,k} - \sqrt{\phi_{w,k}^2/\rho_{gw,k}^2 + 4D_{eT,j,k,1}k_{j,k}}}{2D_{eT,j,k,1}}, \beta''_{j,k,1} = \frac{\phi_{w,k}/\rho_{gw,k} + \sqrt{\phi_{w,k}^2/\rho_{gw,k}^2 + 4D_{eT,j,k,1}k_{j,k}}}{2D_{eT,j,k,1}}$$

- Similar equations apply for O₂

Component Mass Balances Through Wall

Soot oxidation: Products of soot oxidation (CO & NO)

- Soot oxidised by NO₂ according to:



- Component mass balance for NO in soot cake given by:

- $$D_{eT,NO,k,1} \frac{\partial^2 C_{gw,NO,k}}{\partial y^2} - \frac{\psi_{w,k}}{\rho_{gw,k}} \frac{\partial C_{gw,NO,k}}{\partial y} + k_{NO_2,k} C_{gw,NO_2,k} = 0$$

- Term for NO formation depends on solution for NO₂ concentration through soot cake

- Solution for NO concentration:

- $$C_{gw,NO,k} = A_{NO,k,1} + B_{NO,k,1} e^{\beta'_{NO,k,1} y} + k_{NO_2,k} \left(\frac{A_{NO_2,k,1} e^{\alpha''_{NO_2,k,1} y}}{\alpha''_{NO_2,k,1} \psi_{w,k} / \rho_{gw,k} - \alpha''_{NO_2,k,1} D_{eT,NO,k,1}} + \frac{B_{NO_2,k,1} e^{\beta''_{NO_2,k,1} y}}{\beta''_{NO_2,k,1} \psi_{w,k} / \rho_{gw,k} - \beta''_{NO_2,k,1} D_{eT,NO,k,1}} \right)$$

- A similar approach can be used for CO

Component Mass Balances Through Wall

Inert layer / a reactant that does not react in layer

- If component does not react in layer, component mass balance is:

- $$D_{eT,j,k,l} \frac{\partial^2 C_{gw,j,k}}{\partial y^2} - \frac{\phi_{w,k}}{\rho_{gw,k}} \frac{\partial C_{gw,j,k}}{\partial y} = 0$$

- This has solution:

- $$C_{gw,j,k} = A_{j,k,l} + B_{j,k,l} e^{\beta'_{j,k,l} y}$$

- where
$$\beta'_{j,k,l} = \frac{\phi_{w,k}}{\rho_{gw,k} D_{eT,j,k,l}}$$

Component Mass Balances Through Wall

Catalysed layer: Simple (& unlikely) case of first-order, unimolecular kinetics

- For first-order, unimolecular kinetics, rate of formation given by:

- $-R_{j,k}^{(vol)} = S_w k_{mw,j,k} (C_{gw,j,k} - C_{c,j,k}) = k_{j,k}^{(vol)} C_{c,j,k}$

- First term is diffusion to catalyst phase from through-wall flow

- Second term is rate of reaction in catalyst phase

- Rearranging:

- $-R_{j,k}^{(vol)} = \frac{S_w k_{mw,j,k} k_{j,k}^{(vol)} C_{gw,j,k}}{S_w k_{mw,j,k} + k_{j,k}^{(vol)}}$

- Component mass balance:

- $D_{eT,j,k,l} \frac{\partial^2 C_{gw,j,k}}{\partial y^2} - \frac{\phi_{w,k}}{\rho_{gw,k}} \frac{\partial C_{gw,j,k}}{\partial y} - \frac{S_w k_{mw,j,k} k_{j,k}^{(vol)} C_{gw,j,k}}{S_w k_{mw,j,k} + k_{j,k}^{(vol)}} = 0$

- This has solution of the form:

- $C_{gw,j,k} = A_{j,k,l} e^{\alpha_{j,k,l}'''} + B_{j,k,l} e^{\beta_{j,k,l}'''}$

$k_{j,k}^{(vol)}$	= volumetric rate constant
$k_{mw,j,k}$	= mass transfer coefficient
$R_{j,k}^{(vol)}$	= rate per unit volume of catalyst phase
S_w	= external surface area per unit volume for catalyst phase

Component Mass Balances Through Wall

Catalysed layer: Real kinetics

- Make simplifying approximation of single concentration for each species in each element
- Component mass balance:

- $$D_{eT,j,k,l} \frac{\partial^2 C_{gw,j,k}}{\partial y^2} - \frac{\phi_{w,k}}{\rho_{gw,k}} \frac{\partial C_{gw,j,k}}{\partial y} + S_w k_{mw,j,k} (\overline{C_{c,j,k}} - C_{gw,j,k}) = 0$$

- Use mass transfer term for diffusion of reactant/product to catalyst
 - Have used single, representative concentration for catalyst phase, $\overline{C_{c,j,k}}$
 - Result is linear, second-order differential equation
- Solution for concentration through layer is:
 - $$C_{gw,j,k} = A_{j,k,l} e^{\alpha_{j,k,l} y} + B_{j,k,l} e^{\beta_{j,k,l} y} + \overline{C_{c,j,k}}$$

Continuity Between Layers

- Between layers convective and diffusive fluxes continuous:

- $C_{gw,j,k}|_{y_{l,l-1}} = C_{gw,j,k}|_{y_{l,l}}$

- $D_{eT,j,k,l-1} \frac{\partial C_{gw,j,k}}{\partial y} \Big|_{y_{l,l-1}} = D_{eT,j,k,l} \frac{\partial C_{gw,j,k}}{\partial y} \Big|_{y_{l,l}}$

- Similarly, for interface between inlet channel and soot cake:

- Concentration/convection continuity included in inlet channel component mass balance

- $k_{mi,j,k} \left(\frac{[x_{gi,j,k-1} C_{Ti,k-1} + x_{gi,j,k} C_{Ti,k}]}{2} - C_{gw0,j,k} \right) = -D_{eT,j,k,1} \frac{\partial C_{gw,j,k}}{\partial y} \Big|_{y=0}$

- Similar equations apply for outlet channel

Putting it All Together: Solution of Equations

- Have set of linear simultaneous equations
- If have m layers, for each species and each axial element have:
 - Unknowns:
 - Concentration in inlet and outlet channels 2
 - Two arbitrary constants per layer 2m
 - Equations:
 - Component mass balance for inlet and outlet channel 2
 - Continuity of diffusive flux between each channel and wall 2
 - Continuity of concentration and diffusive flux between layers 2(m-1)
 - Total: 2m+2 unknowns & equations – therefore can solve
- Write equations in matrix form ($\mathbf{GH} = \mathbf{J}$) and solve for the unknowns ($\mathbf{H} = \mathbf{G}^{-1}\mathbf{J}$)

Solution of Simultaneous Equations

Solve for each species in each axial element

Write system of simultaneous equations as $\mathbf{GH} = \mathbf{J}$; solve for unknowns in \mathbf{H}

$\mathbf{G} =$

$$= \begin{pmatrix} d_{i,k}^2 \phi_{i,k} / M + p_i k_{mi,j,k} C_{Ti,k} \delta z / 2 & -(p_i k_{mi,j,k} - 4\psi_{w,k} / \rho_{gw,k}) \delta z & -(p_i k_{mi,j,k} - 4\psi_{w,k} / \rho_{gw,k}) \delta z & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ k_{mi,j,k} C_{Ti,k} / 2 & -k_{mi,j,k} + D_{eT,j,k,1} \alpha_{j,k,1}'' & -k_{mi,j,k} + D_{eT,j,k,1} \beta_{j,k,1}'' & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\exp(\alpha_{j,k,1}'' \delta_1) & -\exp(\beta_{j,k,1}'' \delta_1) & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -D_{eT,j,k,1} \alpha_{j,k,1}'' \exp(\alpha_{j,k,1}'' \delta_1) & -D_{eT,j,k,1} \beta_{j,k,1}'' \exp(\beta_{j,k,1}'' \delta_1) & 0 & D_{eT,j,k,2} \beta_{j,k,2}' & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & -\exp(\beta_{j,k,2}' \delta_2) & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -D_{eT,j,k,2} \beta_{j,k,2}' \exp(\beta_{j,k,2}' \delta_2) & D_{eT,j,k,3} \alpha_{j,k,3} & D_{eT,j,k,3} \beta_{j,k,3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\exp(\alpha_{j,k,3} \delta_3) & -\exp(\beta_{j,k,3} \delta_3) & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -D_{eT,j,k,3} \alpha_{j,k,3} \exp(\alpha_{j,k,3} \delta_3) & -D_{eT,j,k,3} \beta_{j,k,3} \exp(\beta_{j,k,3} \delta_3) & D_{eT,j,k,4} \alpha_{j,k,4} & D_{eT,j,k,4} \beta_{j,k,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -(p_o k_{mo,j,k} + 4\psi_{w,k} / \rho_{gw,k}) \exp(\alpha_{j,k,4} \delta_4) \delta z & -(p_o k_{mo,j,k} + 4\psi_{w,k} / \rho_{gw,k}) \exp(\beta_{j,k,4} \delta_4) \delta z & d_o^2 \phi_{o,k} / M + p_o k_{mo,j,k} C_{To,k} \delta z / \gamma & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -(k_{mo,j,k} + D_{eT,j,k,4} \alpha_{j,k,4}) \exp(\alpha_{j,k,4} \delta_4) & -(k_{mo,j,k} + D_{eT,j,k,4} \beta_{j,k,4}) \exp(\beta_{j,k,4} \delta_4) & k_{mo,j,k} C_{To,k} / \gamma & 0 \end{pmatrix}$$

$$\mathbf{H} = \begin{pmatrix} x_{gi,j,k} \\ A_{j,k,1} \\ B_{j,k,1} \\ A_{j,k,2} \\ B_{j,k,2} \\ A_{j,k,3} \\ B_{j,k,3} \\ A_{j,k,4} \\ B_{j,k,4} \\ x_{go,j,k} \end{pmatrix}$$

$$\mathbf{J} = \begin{pmatrix} (d_{i,k-1}^2 \phi_{i,k-1} / M - p_i k_{mi,j,k} C_{Ti,k-1} \delta z / 2) x_{gi,j,k-1} + (p_i k_{mi,j,k} - 4\psi_{w,k} / \rho_{gw,k}) T_1 \delta z \\ k_{mi,j,k} (T_1 - x_{gi,j,k-1} C_{Ti,k-1} / 2) - D_{eT,j,k,1} D_1 \\ T_2 \\ D_{eT,j,k,1} D_2 \\ -C_{c3} \\ 0 \\ C_{c3} - C_{c4} \\ 0 \\ (d_o^2 \phi_{o,k-1} / M - p_o k_{mo,j,k} C_{To,k-1} \delta z / \gamma) x_{go,j,k-1} + (p_o k_{mo,j,k} + 4\psi_{w,k} / \rho_{gw,k}) C_{c4} \delta z \\ k_{mo,j,k} (C_{s4} - x_{go,j,k-1} C_{To,k-1} / \gamma) \end{pmatrix}$$

Catalyst Phase Component Mass Balance

- Including diffusion between through-wall flow and catalyst phase enables calculation of rates of reaction to be separated from rest of mass balances – *a key simplification*
- For an element of volume in catalyst phase, component mass balance:

$$\underbrace{\epsilon_c \frac{\partial C_{c,j,k}}{\partial t}}_{\text{Accumulation}} = \underbrace{S_w k_{mw,j,k} (C_{gw,j,k} - C_{c,j,k})}_{\text{Diffusion to catalyst phase}} + \underbrace{R_{j,k}^{(vol)}}_{\text{Rate}}$$

- Integrate this over volume of catalyst phase & scale for whole filter:

$$(1 - \epsilon_{PF}) f_c \epsilon_c \frac{\partial \overline{C_{c,j,k}}}{\partial t} = 2d\rho_{cell} S_w k_{mw,j,k} \int_0^{\delta_c} (C_{gw,j,k} - \overline{C_{c,j,k}}) dy + S_a R_{j,k}$$

- Have representative concentration in catalyst phase, $\overline{C_{c,j,k}}$; evaluate rate ($R_{j,k}$) at this
 - Exact if $C_{c,j,k} \rightarrow 0$ (case if diffusion to catalyst limiting), otherwise an approximation

- Substitute solution for $C_{gw,j,k}$ and evaluate integral:

$$\bullet \quad (1 - \epsilon_{PF}) f_c \epsilon_c \frac{\partial \overline{C_{c,j,k}}}{\partial t} = 2d\rho_{cell} S_w k_{mw,j,k} \left(\frac{A_{j,k,c}}{\alpha_{j,k,c}} (e^{\alpha_{j,k,c} \delta_c} - 1) + \frac{B_{j,k,c}}{\beta_{j,k,c}} (e^{\beta_{j,k,c} \delta_c} - 1) \right) + S_a R_{j,k}$$

f_c = fraction of wall that is catalyst
 $R_{j,k}^{(vol)}$ = volumetric rate
 $R_{j,k}$ = rate per unit mass catalyst
 ϵ_c = porosity of catalyst phase
 ϵ_{PF} = open frontal area
 δ_c = thickness of catalyst layer

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Simulation Conditions and Parameters

- Simulations run for:
 - 118.4×152.4mm (4.66×6in), 300/8 symmetric filter
 - Wall has porosity 50%, mean pore diameter 16μm
- Three locations for catalyst phase:
 - Throughout whole thickness of filter wall, top half of wall, bottom half of wall
- Mass transfer coeffⁿ for diffusion between inlet channel & wall increases with wall flow
 - $Sh_i = Sh_0 + 0.60Pe_W - 0.143Re_W$ (Bissett, Kostoglou, Konstandopoulos, Chem. Eng. Sci. 84, 255-265 (2012))
 - Otherwise, inlet channel concentration increases along channel at high flow
- Surface area per unit volume for diffusion to catalyst, S_w , assumed to be equated to surface area of pores in the wall divided by wall volume of wall
 - Assumes all pores are lined by catalyst

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- 04** What should the concentration of gas convecting out of the inlet channel be?

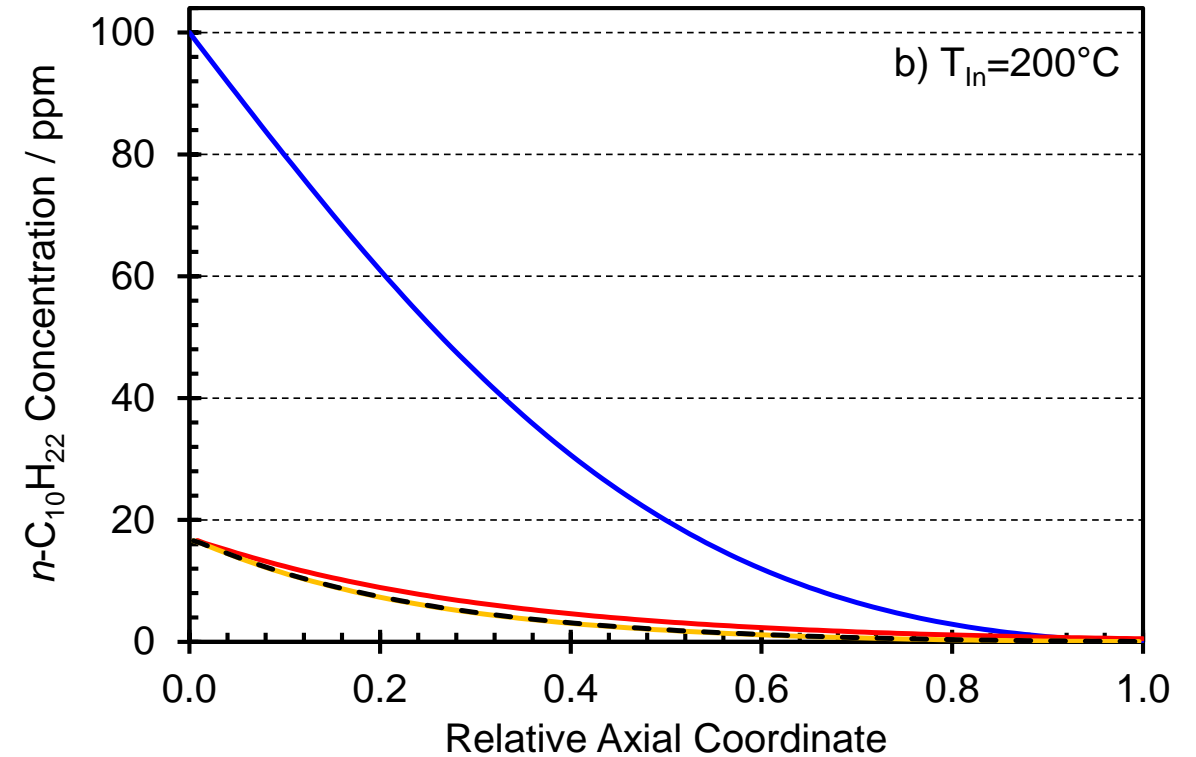
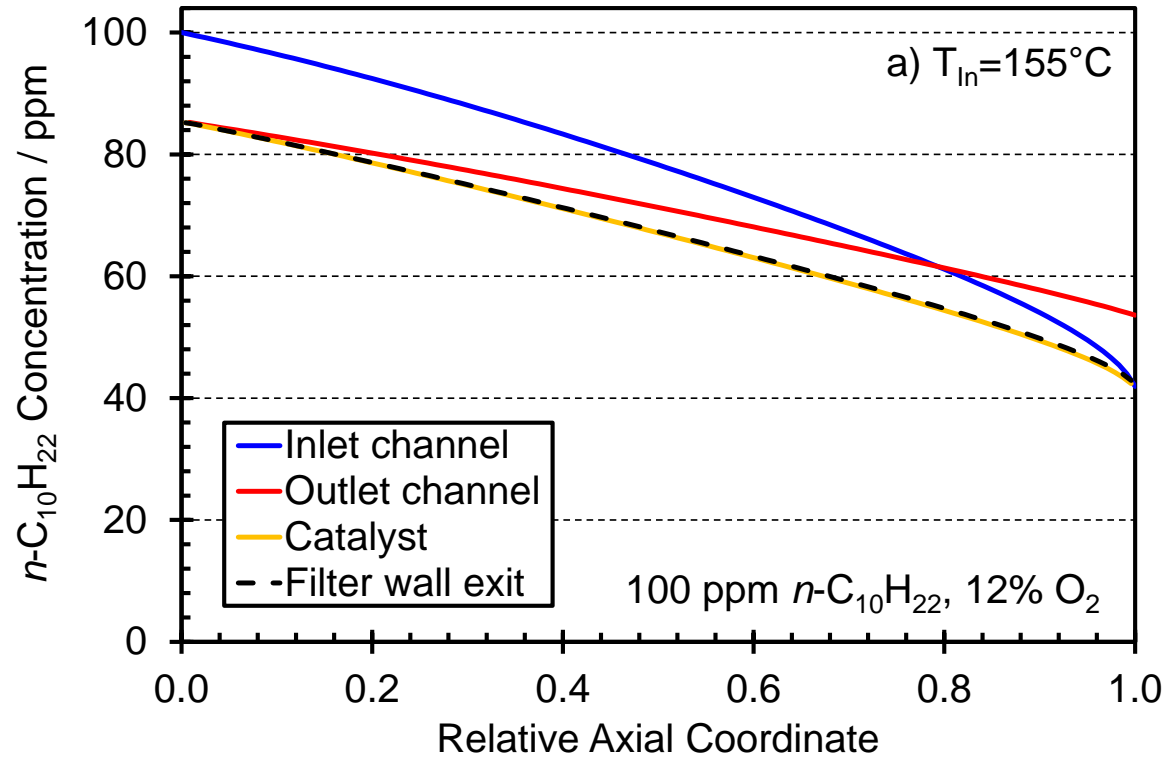
- 05** Example simulations: Oxidation of gaseous components

- 06** Example simulations: Soot oxidation

- 07** Summary / Conclusions

Predicted Axial Profiles for $n\text{-C}_{10}\text{H}_{22}$ Oxidation

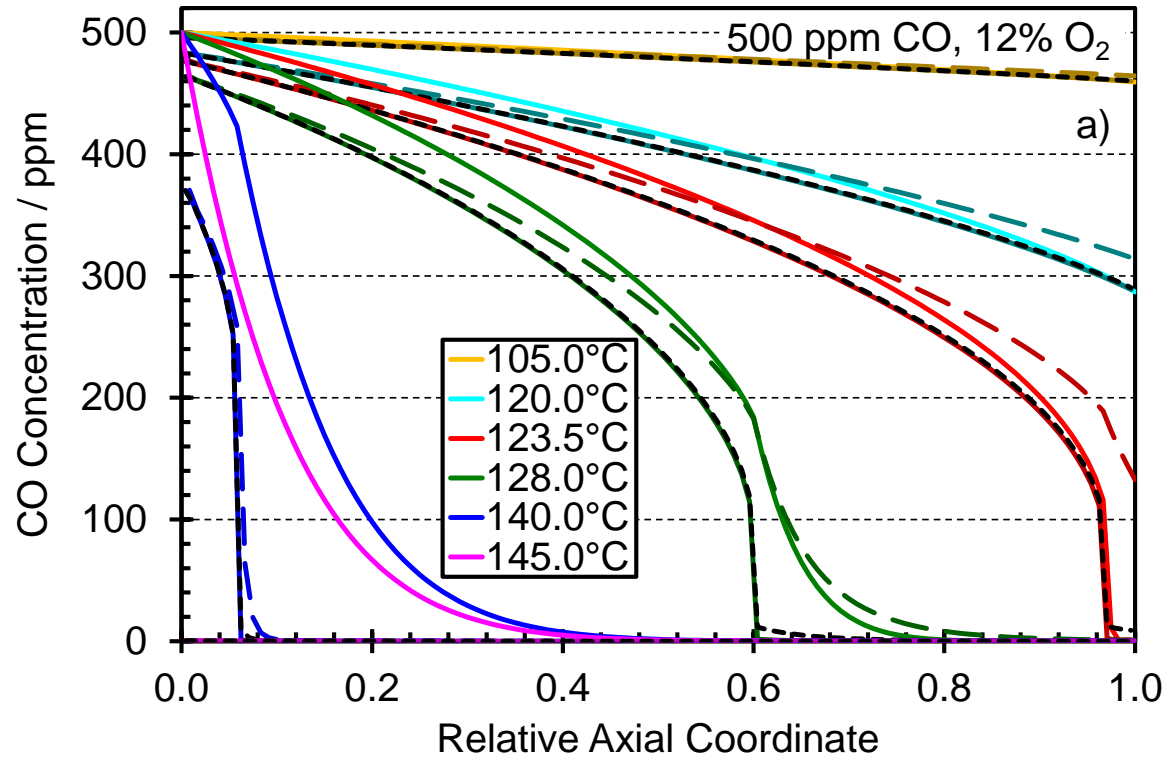
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- Change in concentration across wall due to reaction; this increases with temperature
- Concentration decreases along inlet channel due to diffusion of $\text{C}_{10}\text{H}_{22}$ from channel to wall
- Concentration in outlet channel result of mixing of gas passing along channel and gas flowing in from wall, plus diffusion

Mass flow 0.015 kg s^{-1} , catalyst throughout wall

Predicted Axial Profiles for CO Oxidation



Inlet channel: Solid line
 Outlet channel: Darker line, long dashes
 Catalyst phase: Darker, solid line
 Filter wall exit: Black line, short dashes

0.015 kg s⁻¹, catalyst throughout wall

- Very different behaviour from $n\text{-C}_{10}\text{H}_{22}$
- Strongly self-inhibited reaction exhibits multiple state states
- Sharp change from kinetic control to transported limited regime
 - Concentration in catalyst phase plumes to practically zero at this transition
- In kinetic control region:
 - Curve is concave: reaction becomes faster CO concentration falls due to self-inhibition
 - See decrease in concentration across wall

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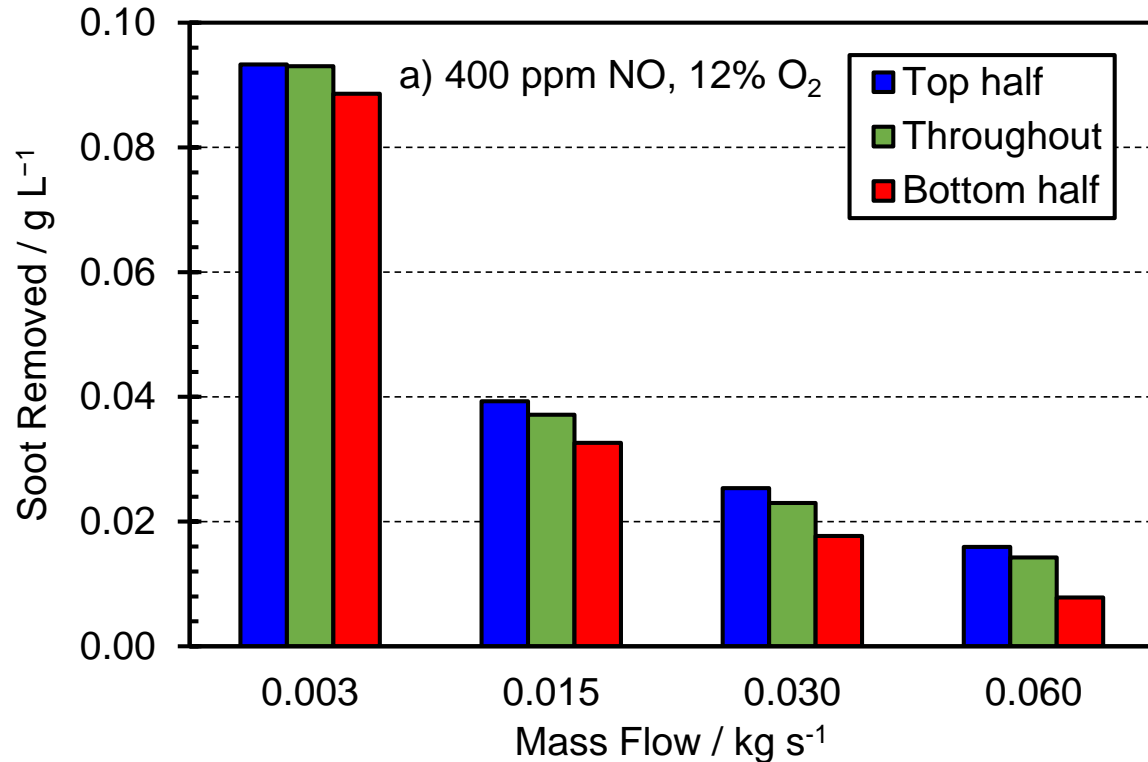
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Soot Oxidation: "NO-Only" Feed

Model prediction

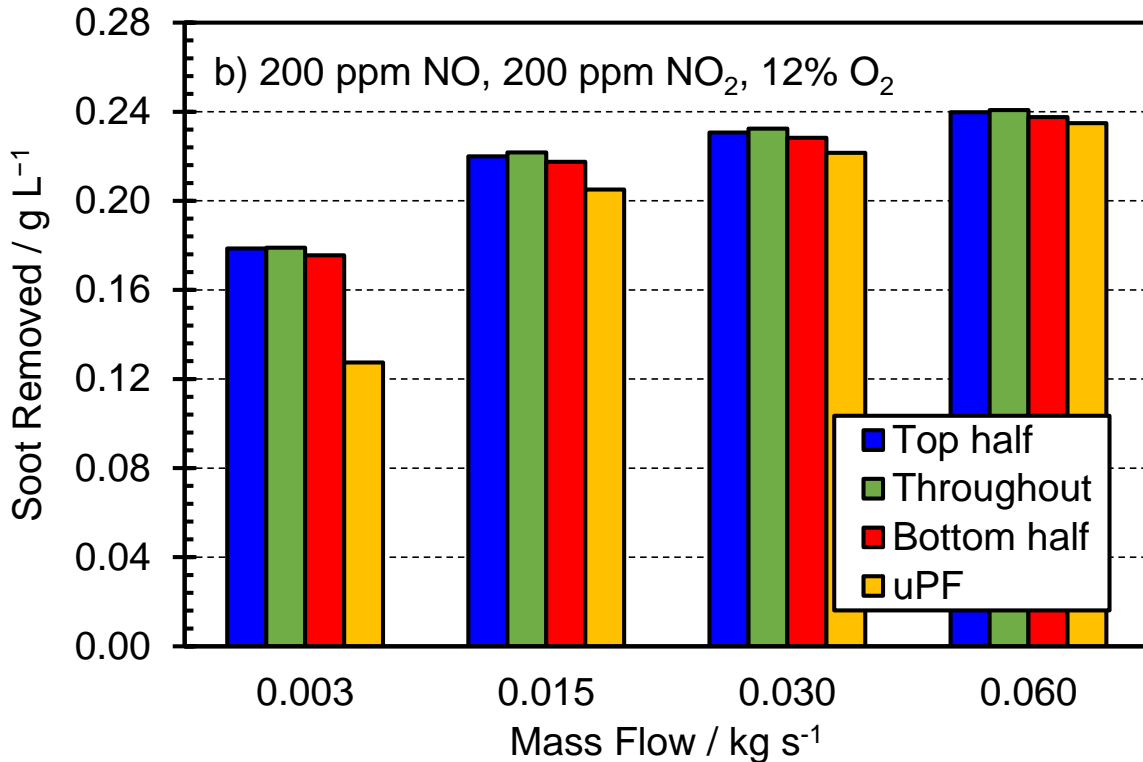


300°C inlet temperature
Initial soot loading 6 g L⁻¹
Simulate for 2000 s

- No NO₂ in feed, so reliant on NO₂ generated on catalyst for soot oxidation
- Soot oxidation favoured by:
 - Low mass flow
 - Lower flow for NO₂ to diffuse against
 - Increases residence time in catalyst and soot cake
 - Proximity of catalyst to soot cake
 - Top half > throughout > bottom half
 - Means shorter diffusion distance

Soot Oxidation: NO+NO₂ Feed

Model prediction



300°C inlet temperature
Initial soot loading 6 g L⁻¹
Simulate for 2000 s

- Faster soot oxidation when NO₂ fed
- Mass flow trend reversed compared to NO-only feed
 - Increasing mass flow increases supply of oxidant to soot
 - More important effect than reduction in contact time
- Catalyst coating still has advantage over uPF
 - This decreases with increasing mass flow
- Soot oxidation increases with proximity of catalyst to soot cake
 - But smaller effect than NO-only case

Outline

- 01** Concept

- 02** Model description

- 03** Simulation conditions and parameters

- 04** Example simulations: Oxidation of gaseous components

- 05** Example simulations: Soot oxidation

- 06** Summary / Conclusions

Summary 1

- Simplified framework for modelling coated particulate filters
 - Avoids the need to discretise in through-wall direction
 - By making approximations/assumptions obtain set of linear simultaneous equations for each species in each axial element
 - Key assumptions:
 - Assume all wall & cake layers are slabs/cuboids – neglect taper on soot and ash cakes
 - Single concentration for each species in each axial element

Summary 2: How Successful is Modelling Approach?

- Good:
 - Plausible predictions
 - Predict differences with through-wall catalyst location
 - Approximation of single concentration for each species in an axial element helped by the fact that reaction is spread along the length of the filter
- However, inevitably a model is always a simplification
 - Distribution of reaction (& concentrations) through wall is approximated