Catalytic Combustion

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Scientific Background

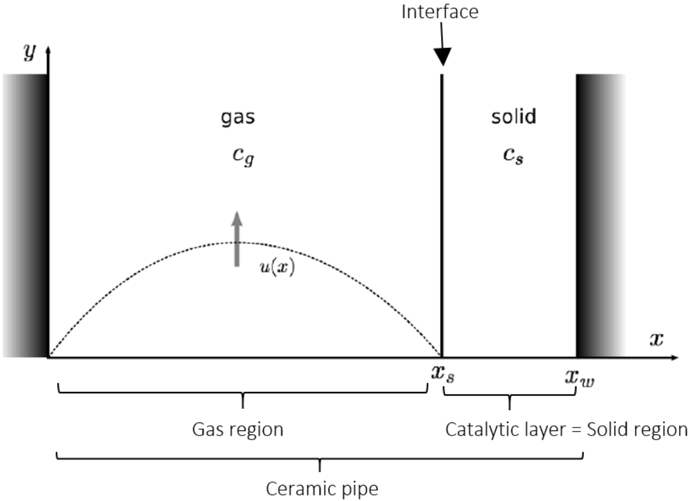
Catalytic combustion: Catalytic combustion is an air purification technique to eliminate a certain type of pollutant substances called VOCs (volatile organic compounds).

It consists of a reaction through which the volatile polluting substances present in the gaseous stream are burned.

Scientific Background

- **Our Model**: A reactor consisting of a ceramic pipe where one of the walls is covered by a thin solid catalytic layer is studied.
- **Mechanism**: While the gas is flowing through the pipe, the pollutant substance present in the gas react with the thin layer developing thermal energy.

Scientific Background



Mathematical Model - PDE and ODE

Coupled PDE-ODE model along the wall of catalytic layer

- **Gas region (PDE)**

$$u(x)\frac{\partial c_g}{\partial y} - D_g \frac{\partial^2 c_g}{\partial x^2} = 0, \quad 0 < x < x_s, \quad y > 0,$$

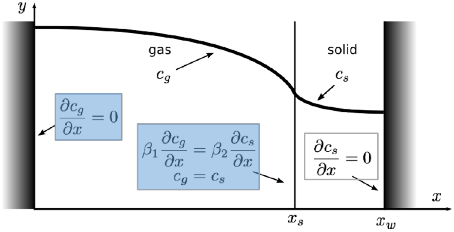
$$\text{where} \quad u(x) = u_{max}\left(1 - 4\left(\frac{x}{x_s} - \frac{1}{2}\right)^2\right)$$

- **Solid region (ODE)**

$$D_s \frac{d^2 c_s}{dx^2} - k c_s = 0, \quad x_s < x < x_w$$

Initial condition

$$c_g(x,0) = c_0, \quad 0 < x < x_s$$



Boundary conditions

- Left wall: $x = 0$

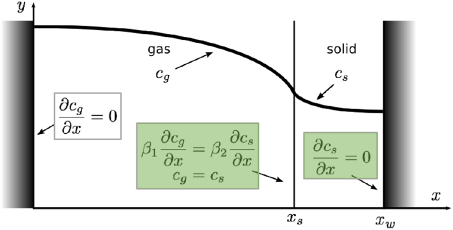
$$\frac{\partial c_g}{\partial x}(0,y) = 0, \quad y > 0$$

- Interface (shared with ODE): $x = x_s$

$$\beta_1 \frac{\partial c_g}{\partial x}(x_s,y) = \beta_2 \frac{dc_s}{dx}(x_s,y), \quad c_g(x_s,y) = c_s(x_s,y), \quad y > 0$$

Initial condition

$$c_s(x,0) = 0, \quad x_s < x < x_w$$



Boundary conditions

- Right wall: $x = x_w$

$$\frac{dc_s}{dx}(x_w, y) = 0, \quad y > 0$$

- Interface (shared with PDE): $x = x_s$

$$\beta_1 \frac{\partial c_g}{\partial x}(x_s, y) = \beta_2 \frac{dc_s}{dx}(x_s, y), \quad c_g(x_s, y) = c_s(x_s, y), \quad y > 0$$

Mathematical Model - Limitations

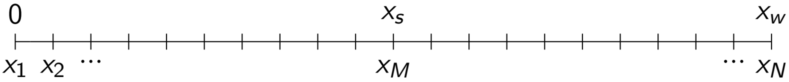
Discretization limitations

- **PDE**: MoL $\rightarrow$ discretization of x space derivatives with FDM $\rightarrow$ stiff ODE system $\rightarrow$ implicit Euler to solve ODE
  $\Rightarrow$ <u>1st order</u> accuracy
- **ODE**: FDM with central differences
  $\Rightarrow$ <u>2nd order</u> accuracy
- **BCs**: Forward and backward differences
  $\Rightarrow$ <u>1st order</u> accuracy

Other limitations

- We assume that the process takes place isothermally, i.e. under constant temperature.

x-axis discretization



We have:

- Gas Region $\in [x_1, x_M)$
- Solid Region $\in (x_M, x_N]$.

The step size is the same for both regions:

$$h_x = \frac{x_s}{M-1}$$
$$h_x = \frac{x_w - x_s}{N-M}$$

Gas region PDE - MoL and derivatives discretization

- Discretization using **Method of lines** for Parabolic PDE in each x_j point approximating $c_g(x_j) \approx c_g^{(j)}$
- Implicit Euler for ODE system with constant step-size h_y satisfying the stability condition
- Approximation of second derivative using central difference:

$$\frac{\partial^2 c_g}{\partial x^2} \approx \frac{c_g^{(j+1)} - 2c_g^{(j)} + c_g^{(j-1)}}{h_x^2}$$

- Approximation of first derivative for BC with forward and backward differences:

$$\frac{\partial c_g}{\partial x} \approx \frac{c_g^{(j+1)} - c_g^{(j)}}{h_x}, \qquad \frac{\partial c_g}{\partial x} \approx \frac{c_g^{(j)} - c_g^{(j-1)}}{h_x}$$

Gas region PDE - Discretization

- **PDE Equation**:

$$\frac{\partial c_g}{\partial y} = \frac{D_g}{u(x)} \frac{c_g^{(j+1)} - 2c_g^{(j)} + c_g^{(j-1)}}{h_x^2}$$

- **Boundary Condition** (Zero Flux Neumann Condition) at the grid point $x_1 = 0$, for $y > 0$:

$$\frac{\partial c_g}{\partial x}(0, y) = \frac{c_g^{(2)} - c_g^{(1)}}{h_x} = 0, \quad \Leftrightarrow \quad c_g^{(1)} = c_g^{(2)}$$

- **Boundary Condition** at x_s

$$\beta_1 \frac{c_g^{(M)} - c_g^{(M-1)}}{h_x} = \beta_2 \frac{c_s^{(M+1)} - c_s^{(M)}}{h_x}, \quad c_g^{(M)} = c_s^{(M)}$$

$$(\beta_1 + \beta_2) c_g^{(M)} - \beta_1 c_g^{(M-1)} - \beta_2 c_s^{(M+1)} = 0$$

Gas region PDE - Matrix Formulation

We get the following matrix:

$$P = \frac{D_g}{u(i)h_x^2} \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix}$$

- $P \in \mathbb{R}^{M \times M}$.
- Implicit Euler $\quad c_g^{(j,n+1)} = c_g^{(j,n)} + h_y P c_g^{(j,n+1)}$

$$\Rightarrow (I - h_y P) c_g^{(j,n+1)} = c_g^{(j,n)}$$

- The first and last rows of the matrix are changed later according to the boundary conditions.

Solid region ODE - FDM

- Discretization using **Finite Difference Method** in each x_j point approximating $c_s(x_j) \approx c_s^{(j)}$;
- Approximation of second derivative using central difference:

$$\frac{d^2 c_s}{dx^2} \approx \frac{c_s^{(j+1)} - 2c_s^{(j)} + c_s^{(j-1)}}{h_x^2}$$

- Approximation of first derivative (for BC) using backward difference:

$$\frac{dc_s}{dx} \approx \frac{c_s^{(j)} - c_s^{(j-1)}}{h_x}$$

Solid region ODE - Discretization

- **ODE Equation**:

$$D_s \frac{c_s^{(j+1)} - 2c_s^{(j)} + c_s^{(j-1)}}{h_x^2} - kc_s^{(j)} = 0$$

- **Boundary Condition** (Zero Flux Neumann Condition) at x_w which corresponds to the $N-th$ point of the grid:

$$\frac{dc_s}{dx}(x_w, y) = \frac{c_s^{(N)} - c_s^{(N-1)}}{h_x} = 0, \quad \Leftrightarrow \quad c_s^{(N)} = c_s^{(N-1)}$$

- **Boundary Condition** at x_s interface discretized as shown above.

Solid region ODE - Matrix Formulation

We get the following matrix:

$$O = \frac{D_s}{h_x^2} \begin{pmatrix} (-2 - k\frac{D_s}{h_x^2}) & 1 & & & \\ 1 & (-2 - k\frac{D_s}{h_x^2}) & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & (-2 - k\frac{D_s}{h_x^2}) & 1 \\ & & & 1 & (-2 - k\frac{D_s}{h_x^2}) \end{pmatrix}$$

- $O \in \mathbb{R}^{N-M \times N-M}$.

Differential Algebraic System DAE - A matrix

$$
A = \left(\begin{array}{ccc|ccc}
\boxed{-1} & \boxed{1} & 0 & 0 & \dots & 0 \\
\multicolumn{3}{c|}{\textbf{I-hyP}} & 0 & \dots & 0 \\
 & \boxed{-1} & \boxed{3} & \boxed{-2} & 0 \dots & 0 \\
\hline
0 & \dots 0 & \boxed{\frac{D_s}{h_x^2}} & \multicolumn{3}{c}{\mathbf{O}} \\
0 & \dots & 0 & & \boxed{-1} & \boxed{1}
\end{array} \right)
$$

- $A \in \mathbb{R}^{N \times N}$
- Green elements: PDE BC at $x = 0$
- Blue elements: BC at the interface $x = x_s$
- Pink element: discretization at $c_s^{(M+1)}$, for $c_s^{(M)} = c_g^{(M)}$
- Yellow elements: ODE BC at $x = x_w$

DAE systems

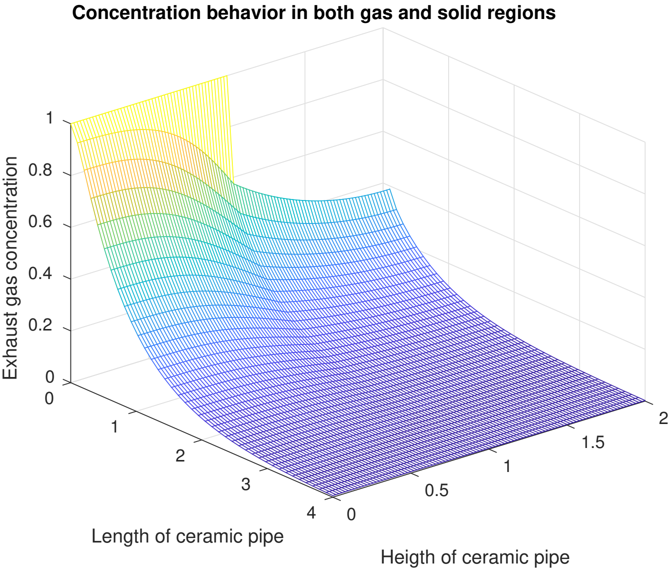
We consider the following system:

$$A\mathbf{c}^{(\mathbf{k})} = \mathbf{b}^{(\mathbf{k-1})},$$
$$\mathbf{c} = (\mathbf{c}_g, \mathbf{c}_s), \qquad \mathbf{b} = (\mathbf{c_g}, \mathbf{0})$$

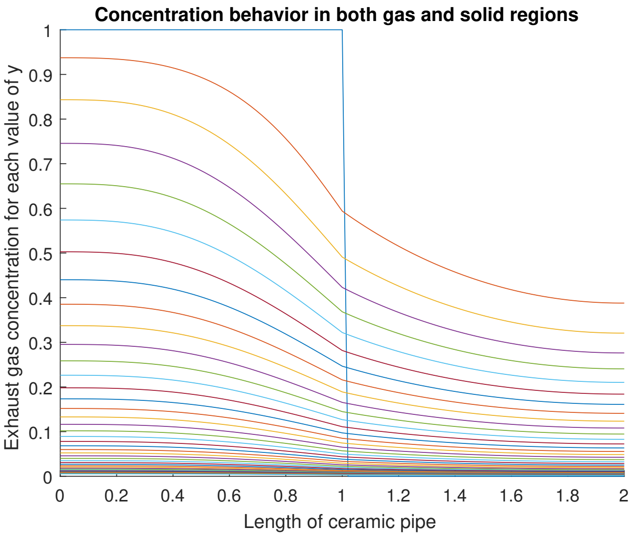
- A sparse tridiagonal matrix.
- The solution is built iteratively.
- The $\mathbf{c}^{(\mathbf{k})}$ is our unknown vector of concentration.
- The first one corresponds to the initial condition, then at each step between 0 and y_{max} we calculate the current solution as $A \setminus c$ and update the $\mathbf{C}$ matrix, collecting all the solutions.
- $C \in \mathbb{R}^{N \times length(y)}$

Numerical Results - Standard Values

- $h_y = 0.1$
- $x_s = 1$
- $x_w = 2$
- $D_g = 1$
- $D_s = 1$
- $k = 1$
- $\beta_1 = 1$
- $\beta_2 = 2$
- $c_0 = 1$
- $u_{max} = 1$
- $M = 51$
- $y_{max} = 4$

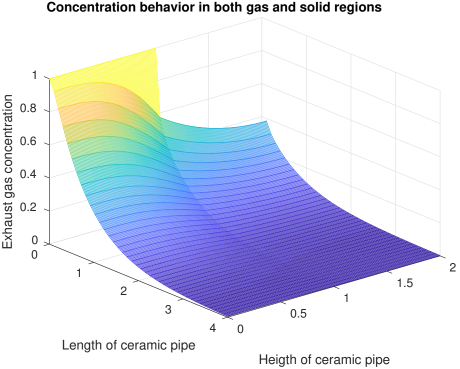


Numerical Results - Standard Values

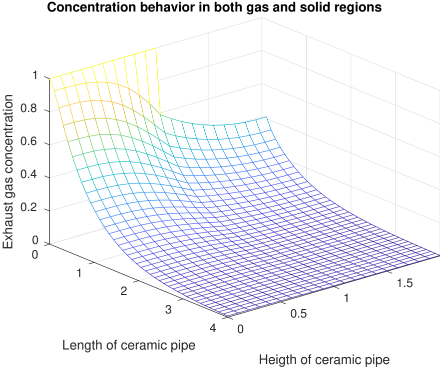


Numerical Results - Changing M

$M = 101$

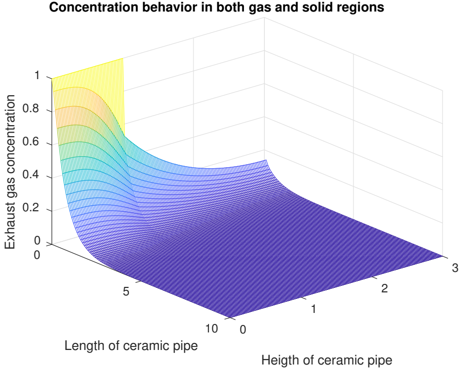


$M = 11$

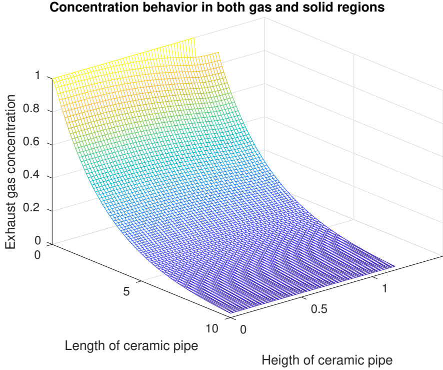


Numerical Results - Changing x_w

$x_w = 3$

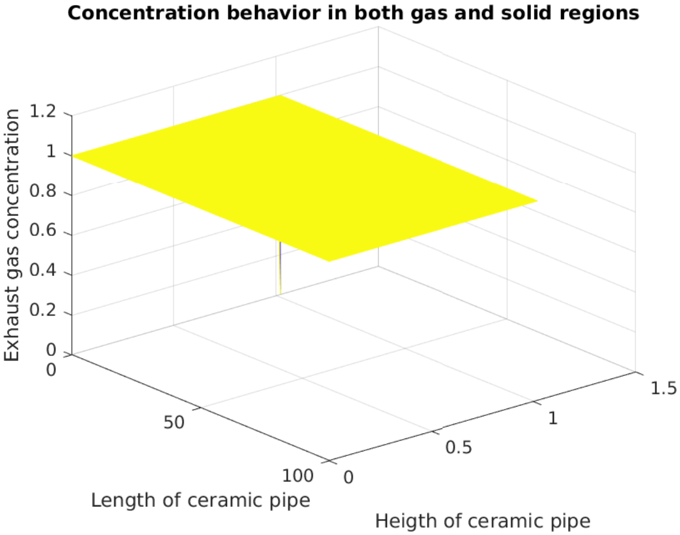


$x_w = 1.16$



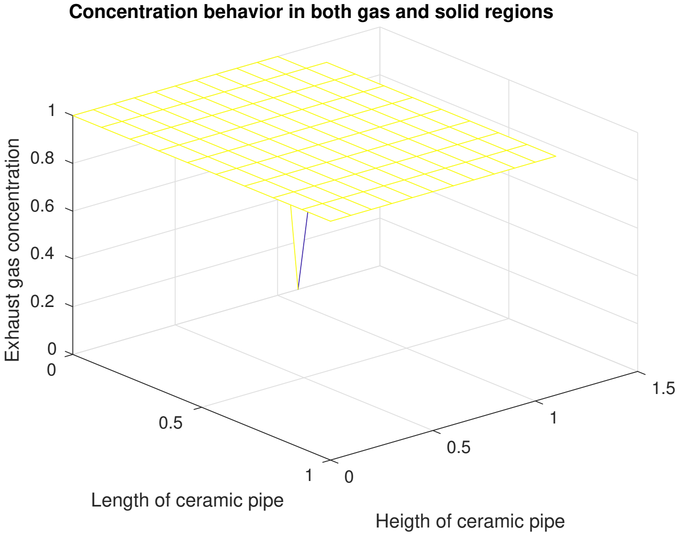
Numerical Results - No Catalysator

- $x_w = 1.02$
- $h_y = 1$



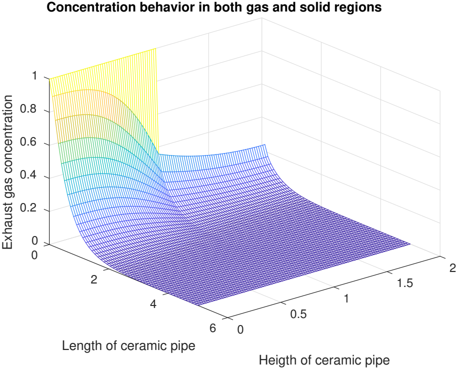
Numerical Results - No Catalysator

- $x_w = 1.1$
- $N = 11$

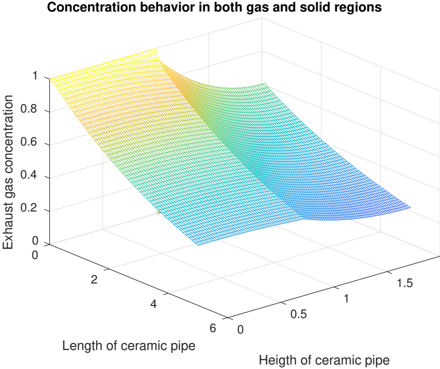


Numerical Results - Changing β_2

$\beta_2 = 5$

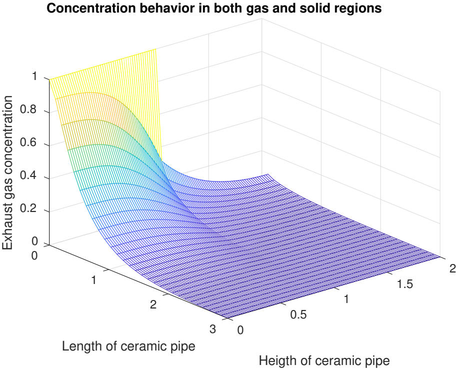


$\beta_2 = 0.2$

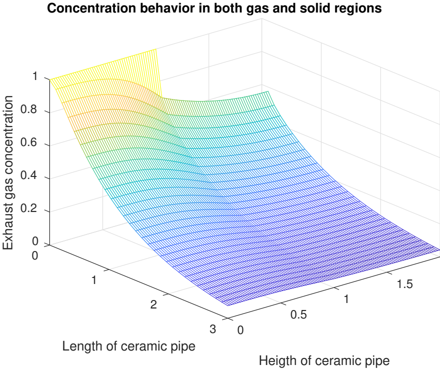


Numerical Results - Changing k

$k = 5$

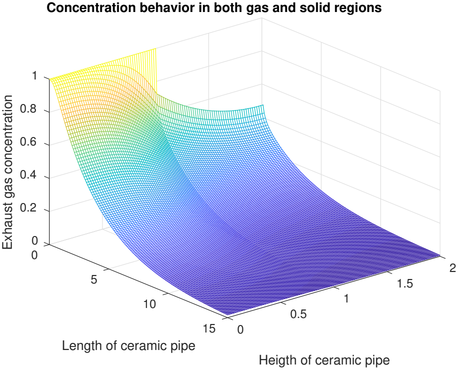


$k = 0.5$



Numerical Results - Changing u_{max}

$u_{max} = 5$



$u_{max} = 0.2$