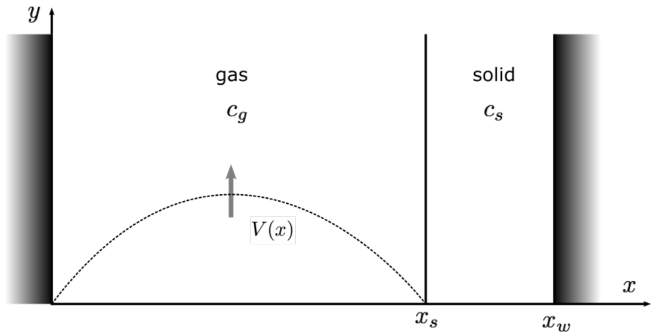
KTH Engineering Sciences

Project
Catalytic combustion



Catalytic combustion is an important application of chemical technology, where environmentally dangerous species can be eliminated in the exhaust gases from e.g. a combustion engine.

In this project we study a reactor consisting of a narrow ceramic pipe of width x_s and length L [m], where one of the walls is covered by a solid catalytic layer of width $x_w - x_s$. The pipe contains a fuel gas, the flow of which is laminar. Therefore its velocity profile $V(x)$ [m/s] can be considered to be parabolic. The gas is in contact with the catalytic layer and diffuses into the solid region, where it undergoes a catalytic reaction and is consumed while developing thermal energy. To simplify the conditions, however, we assume that the process takes place isothermally, i.e. under constant temperature.

We use a 2D mathematical model for the profiles of the fuel gas concentration in the gas region $c_g(x, y)$ and in the solid region $c_s(x, y)$ [kg/m^3]. The model is a coupled PDE-ODE system, where the PDE is valid in the gas region,

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

and the ODE is valid in the solid region

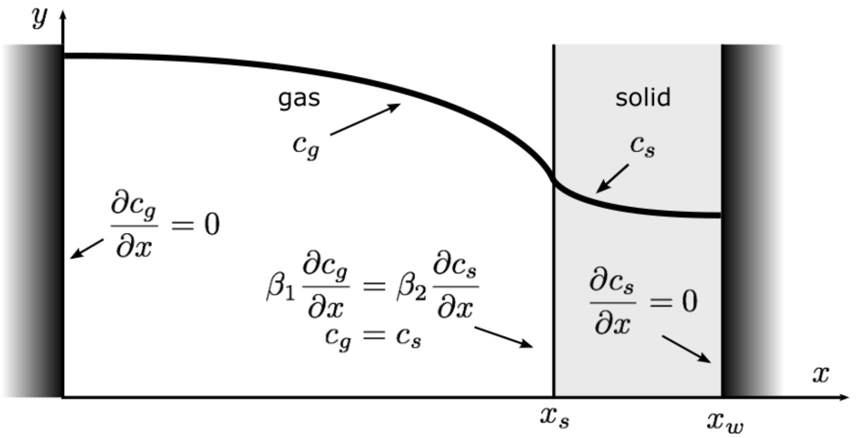
$$D_s\frac{d^2 c_s}{dx^2} - kc_s = 0, \quad x_s < x < x_w, \quad 0 < y < L.$$

These equations are given by the mass balances for the fuel gas. The coefficients D_g and D_s [m^2/s] are diffusion coefficients and k [s^{-1}] is the catalytic reaction rate. The coupling between the PDE and the ODE takes place through interface conditions at $x = x_s$, where the gas meets the catalytic layer,

$$c_g(x_s, y) = c_s(x_s, y), \qquad D_g\frac{\partial c_g}{\partial x}(x_s, y) = D_s\frac{dc_s}{dx}(x_s, y), \qquad 0 < y < L.$$

The boundary conditions at the outer walls $x = 0$ and $x = x_w$ are

$$\frac{\partial c_g}{\partial x}(0, y) = 0, \quad \frac{dc_s}{dx}(x_w, y) = 0, \quad 0 < y < L.$$



The initial condition is

$$c_g(x, 0) = C_0, \quad 0 < x < x_s.$$

Note that no initial condition for c_s is needed. The parabolic velocity profile function $V(x)$ is given by

$$V(x) = V_{\max}\left(1 - 4\left[\frac{x}{x_s} - \frac{1}{2}\right]^2\right), \quad 0 < x < x_s.$$

Tasks

1. Rescaling

Introduce the rescaled variables u_g, u_s, τ and z as

$$c_g = u_g C_0, \qquad c_s = u_s C_0, \qquad x = z x_s, \qquad \tau = yL.$$

Rescale the equations to dimensionless form and show that they can be written as

$$\begin{aligned} v(z)\frac{\partial u_g}{\partial \tau} - \eta \frac{\partial^2 u_g}{\partial z^2} &= 0, \qquad z, \tau \in (0, 1), \\ \frac{d^2 u_s}{dz^2} - \gamma u_s &= 0, \quad z \in (1, 1 + w), \quad \tau \in (0, 1). \end{aligned} \tag{1}$$

with boundary and initial conditions given by

$$u_g(z, 0) = 1, \qquad \frac{\partial u_g}{\partial z}(0, \tau) = \frac{\partial u_s}{\partial z}(1 + w, \tau) = 0,$$

for $z, \tau \in (0, 1)$ and the interface conditions

$$u_g(1, \tau) = u_s(1, \tau), \qquad \frac{\partial u_g}{\partial z}(1, \tau) = \alpha \frac{\partial u_s}{\partial z}(1, \tau),$$

for $\tau \in (0, 1)$. Moreover,

$$v(z) = 1 - 4\left(z - \frac{1}{2}\right)^2.$$

Determine the dimensionless numbers η, γ, w and α as functions of x_s, x_w, L, D_s, D_g, k, C_0, $V_{\max}$. In the computations below, start by using the values $\eta = 0.2$, $\gamma = 100$, $\alpha = 0.2$ and $w = 0.3$. Describe a physical setup that corresponds to this case. Note that the model is derived under the assumption that $(x_s/L)^2 \ll \min(1, 1/\eta)$, so it should respect that.

2. Discretization

Discretize the rescaled problem (1) in z, using a uniform discretization $z_j = j\Delta z$ where Δz should be chosen such that $z_M = 1$ and $z_{M+N} = 1 + w$ for some integers M, N. Introduce the approximations $u_g^j(\tau) \approx u_g(z_j, \tau)$ and $u_s^j(\tau) \approx u_s(z_{M+j}, \tau)$. Let $\bar{u}(\tau) = u_g^M(\tau) = u_s^0(\tau)$ be the common name for the concentration at the interface point. Use finite differences to approximate the PDE, the ODE, the boundary and the interface conditions. For the interface condition you may use a first order approximation. You will end up with a semi-discretization of the following form

$$\frac{d}{d\tau}\begin{pmatrix} \boldsymbol{u}_g \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} A_1 & \boldsymbol{e}_1 & 0 \\ \boldsymbol{b}_1^T & a & \boldsymbol{b}_2^T \\ 0 & \boldsymbol{e}_2 & A_2 \end{pmatrix}\begin{pmatrix} \boldsymbol{u}_g \\ \bar{u} \\ \boldsymbol{u}_s \end{pmatrix}, \qquad \boldsymbol{u}_g = \begin{pmatrix} u_g^1 \\ \vdots \\ u_g^{M-1} \end{pmatrix}, \quad \boldsymbol{u}_s = \begin{pmatrix} u_s^1 \\ \vdots \\ u_s^{\tilde{N}} \end{pmatrix}, \tag{2}$$

where $\tilde{N}$ is either N or $N-1$ depending on how you treat the rightmost boundary. Note that since $v(0) = 0$ you should avoid including u_g^0 among the unknowns. The subblocks consist of the matrices $A_1 \in \mathbb{R}^{(M-1)\times(M-1)}$, $A_2 \in \mathbb{R}^{\tilde{N}\times\tilde{N}}$ the vectors $\boldsymbol{e}_1, \boldsymbol{b}_1 \in \mathbb{R}^{M-1}$, $\boldsymbol{e}_2, \boldsymbol{b}_2 \in \mathbb{R}^{\tilde{N}}$, and the scalar value a. Derive expressions for these matrix blocks. The semi-discretization (2) is an example of a *differential algebraic system of equations*, or *DAE system*, as not all derivatives are present in the left hand side.

3. Numerical investigations

Compare three different solution methods for the DAE system (2). The methods are described below. What are their advantages and disadvantages? Properties of interest are e.g. computational cost, accuracy, robustness, generalizability, etc.

- The Implicit Euler method.

  For the DAE system (1) the Implicit Euler method is formulated as

$$\begin{pmatrix} \boldsymbol{u}_g^{n+1} \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \boldsymbol{u}_g^{n} \\ 0 \\ 0 \end{pmatrix} + \Delta\tau \begin{pmatrix} A_1 & \boldsymbol{e}_1 & 0 \\ \boldsymbol{b}_1^T & a & \boldsymbol{b}_2^T \\ 0 & \boldsymbol{e}_2 & A_2 \end{pmatrix}\begin{pmatrix} \boldsymbol{u}_g^{n+1} \\ \bar{u}^{n+1} \\ \boldsymbol{u}_s^{n+1} \end{pmatrix}.$$

  Note that this can be further reduced to simply $B\boldsymbol{u}_g^{n+1} = \boldsymbol{u}_g^n$ for a fixed matrix B.

- Regularization together with the Implicit Euler method.

  Here the DAE system is turned into an ODE system by adding a suitably small regularization parameter ε,

$$\frac{d}{d\tau}\begin{pmatrix} \boldsymbol{u}_g \\ \bar{u} \\ \boldsymbol{u}_s \end{pmatrix} = \begin{pmatrix} I & & \\ & \frac{1}{\varepsilon} & \\ & & \frac{1}{\varepsilon}I \end{pmatrix}\begin{pmatrix} A_1 & \boldsymbol{e}_1 & 0 \\ \boldsymbol{b}_1^T & a & \boldsymbol{b}_2^T \\ 0 & \boldsymbol{e}_2 & A_2 \end{pmatrix}\begin{pmatrix} \boldsymbol{u}_g \\ \bar{u} \\ \boldsymbol{u}_s \end{pmatrix}.$$

  This ODE system is then solved by Implicit Euler. If $\varepsilon \ll 1$ the $\bar{u}$ and $\boldsymbol{u}_s$ components will quickly relax to the same values as in (2). (Why?)

  Here you also need to give initial conditions for $\bar{u}$ and $\boldsymbol{u}_s$. You can for instance take $\bar{u} = \boldsymbol{u}_s = 1$, but you can also try other choices. In principle the choice should not matter when $\varepsilon \to 0$, but for finite ε it will matter.

- Analytic reduction together with the Implicit Euler method.

  For a given value of $\bar{u}(\tau) = u_s(1,\tau)$ it is possible to find an analytical expression for $u_s(z,\tau)$ in $1 < z \leq 1+w$. (It satisfies a linear ODE.) Take advantage of this. Show that u_s and $\bar{u}$ can be eliminated from the PDE-ODE system, and that it can be reduced to the following PDE for u_g,

$$v(z)\frac{\partial u_g}{\partial \tau} - \eta\frac{\partial^2 u_g}{\partial z^2} = 0, \quad 0 < z < 1, \quad 0 < \tau < 1,$$

$$\frac{\partial u_g}{\partial z}(0,\tau) = 0, \qquad \frac{du_g}{dz}(1,\tau) + \beta u_g(1,\tau) = 0, \qquad u_g(z,0) = 1,$$

  for some β. Find this β and solve the reduced system with the Implicit Euler method. Note that β is a measure of how effective the catalytic layer is; the larger β, the more gas is removed.

4.Investigations of the solution

Select one of the methods above, and investigate how the solution depends on the different parameters of the problem. Vary the dimensionless parameters and illustrate their effect on the solution, by plotting sequences of curves in the same graph showing the fuel gas concentration u_g and u_s computed with different parameter values. Also define the total amount T of fuel gas in a cross-section of the pipe as

$$T(\tau) = \int_0^1 u_g(z,\tau)dz,$$

and plot T as a function of τ for different parameter choices to see how effective the catalytic layer is at removing the gas. Pinpoint how the parameters should be set for the catalytic layer to work well. Also, think about what your analytical formula for β tells you about how the parameters affect the solution.

Finally, connect back to the physical problem. How do your conclusions translate to the physical dimensions x_w, x_s, the pipe length L, the reaction rate k, the diffusion coefficients D_s, D_g and the gas velocity $V_{\max}$? How should they be chosen to get an effective catalysis process?