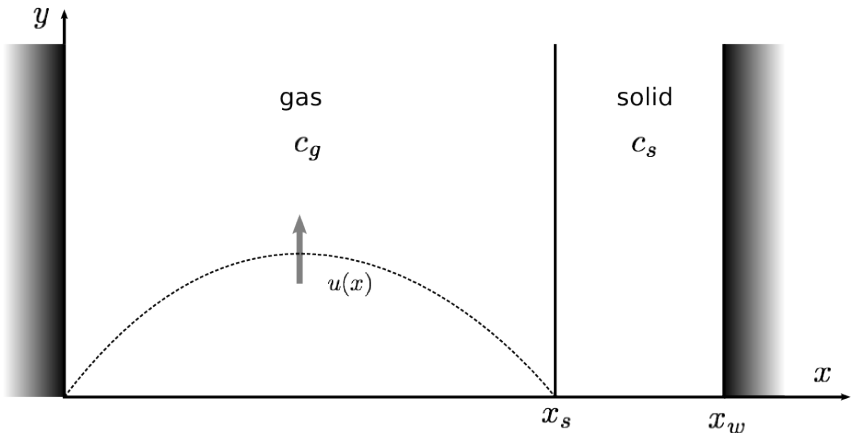
Catalytic Combustion

Numerical solution of a differential algebraic (DAE) system

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 ceramic pipe where one of the walls is covered by a thin solid catalytic layer.

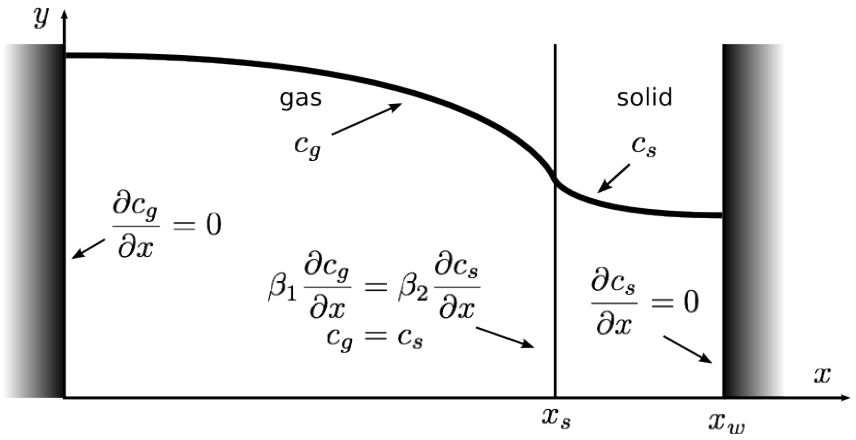


The space between the wall and the catalytic layer, the gas region, contains a fuel gas, the flow of which is laminar. Therefore its velocity profile $u(x)$ can be considered to be parabolic. The gas is transported into the catalytic layer, the solid region, where it undergoes a catalytic reaction and is consumed while developing thermal energy. To simplify the conditions, however, we assume that the process takes place isothermally, i.e. under constant temperature.

The goal of the project is to study a 2D mathematical model of the profiles of the gas concentration in the gas region $c_g(x, y)$ and in the solid region $c_s(x, y)$. The model consists of a coupled PDE-ODE, where the PDE is valid in the gas region and the ODE is valid in the solid region. The coupling between the PDE and the ODE takes place through the boundary conditions given along the wall of the catalytic layer, the interface between the gas region and the solid region. Two mass balances can be formulated for the fuel gas, one for the gas region (1) and one for the solid region (2).

$$u(x)\frac{\partial c_g}{\partial y} - D_g\frac{\partial^2 c_g}{\partial x^2} = 0, \quad 0 < x < x_s, \quad y > 0, \tag{1}$$

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



with boundary conditions at the walls $x = 0$ and $x = x_w$:

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

and boundary conditions at the interface $x = x_s$:

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

with initial conditions

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

and the parabolic velocity profile function $u(x)$

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

This problem contains a number of parameters: $x_s, x_w, D_g, D_s, k, \beta_1, \beta_2, u_{max}$ and c_0 In a test run you can use the values $x_s = 1, x_w = 2, D_g = 1, D_s = 1, k = 1, \beta_1 = 1, \beta_2 = 2, u_{max} = 1, c_0 = 1$, but you can also try to find more realistic values. Finally note that this problem ressembles the interface problem in heat conduction, Example 4.9 in the textbook.

Use the FDM to solve the problem numerically. Make a discretization of the x-interval $[0, x_w]$ into grid points $x_0, x_1, x_2, \ldots, x_M, x_{M+1}, \ldots, x_N$, where $x_1 = 0, x_M = x_s, x_N = x_w$ and the stepsize h_x is constant and the same for both regions: $(M-1)h_x = x_s$ and $(N-M)h_x = x_w - x_s$. Use the MoL, central difference approximation for the second derivative to discretize the PDE (1) and we obtain a system of ODEs with y as independent variable. The ODE (2) is discretized with central differences and an algebraic system of equations is obtained. These two systems, together with discretized boundary conditions, constitute a *differential algebraic system, DAE-system.* A simple way to solve such a system is with Euler's implicit method, constant stepsize h_y, which, however, is only first order in accuracy. Because of that the boundary conditions should also be represented by first order approximations, where Euler's forward difference formula is the simplest.

With the hints given above, structure the problem to a sequence of linear systems of algebraic equations $A\mathbf{c}^{(k)} = \mathbf{b}^{(k-1)}$, that has to be solved for each y-value. Here $\mathbf{c} = (\mathbf{c}_g, \mathbf{c}_s)$ and $\mathbf{b} = (\mathbf{c}_g, \mathbf{0})$ Be careful to check that the number of unknowns and the number of equations are the same in the linear system, hence the matrix A must be quadratic! If the numering of the unknowns is done according to the numbering of the grid points the matrix A will be almost tridiagonal, hence a sparse solver should be used. Plot a sequence of curves in the same graph showing the fuel gas concentration $c_g(x, y)$ and $c_s(x, y)$ as functions of x, for fixed y-values.