Group 2 - Catalytic Combustion

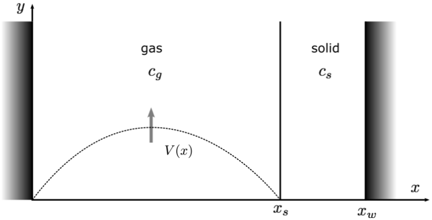
Project SF2520 Applied Numerical Methods

David Ahnlund, Albert Aillet, Max Hollingworth, Rikard Landfeldt

KTH Royal Institute of Technology

Background

- Used to eliminate dangerous compounds in fuel gas
- Catalytic combustion in a pipe
- Parabolic velocity profile due to laminar flow
- Assume constant temperature to simplify



PDE:

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

ODE:

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

- c is the fuel gas concentration $[kg/m^3]$
- D is the diffusion coefficients $[m^2/s]$
- k is the catalytic reaction rate $[s^{-1}]$

Background

Interface:

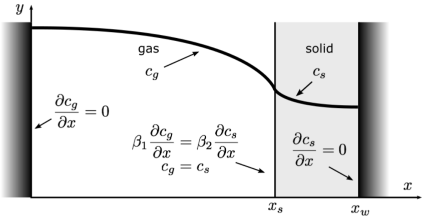
$$c_g(x_s, y) = c_s(x_s, y), \quad D_g \frac{\partial c_g}{\partial x}(x_s, y) = D_s \frac{\partial c_s}{\partial x}(x_s, y), \quad 0 < y < L.$$

BC:

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

IC:

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



Rescaling

Using these rescaled variables:

$$c_g = u_g C_0, \qquad c_s = u_s C_0, \qquad x = z x_s, \qquad y = \tau L$$

And substituting them into the PDE, ODE, BC, IC and Interface Condition:
The PDE becomes:

$$V(zx_s)\frac{\partial(u_g C_0)}{\partial(\tau L)} - D_g \frac{\partial^2(u_g C_0)}{\partial(zx_s)^2} = 0, \qquad 0 < zx_s < x_s, \qquad 0 < \tau L < L$$

$$\Rightarrow V_{max}\left(1 - 4\left[\frac{zx_s}{x_s} - \frac{1}{2}\right]^2\right)\frac{C_0}{L}\frac{\partial u_g}{\partial \tau} - D_g \frac{C_0}{x_s^2}\frac{\partial^2 u_g}{\partial z^2} = 0, \quad 0 < z < 1, \quad 0 < \tau < 1$$

$$\Rightarrow \underbrace{\left(1 - 4\left[z - \frac{1}{2}\right]^2\right)}_{v(z)}\frac{\partial u_g}{\partial \tau} - \underbrace{\frac{D_g L}{V_{max} x_s^2}}_{\eta}\frac{\partial^2 u_g}{\partial z^2} = 0, \quad 0 < z < 1, \quad 0 < \tau < 1$$

Rescaling

The ODE becomes:

$$D_s \frac{d^2(u_s C_0)}{d(zx_s)^2} - k(u_s C_0) = 0, \qquad x_s < zx_s < x_w, \qquad 0 < \tau L < L$$

$$\Rightarrow D_s \frac{C_0}{x_s^2} \frac{d^2 u_s}{dz^2} - kC_0 u_s = 0, \qquad 1 < z < \frac{x_w}{x_s}, \qquad 0 < \tau < 1$$

$$\Rightarrow \frac{d^2 u_s}{dz^2} - \frac{kx_s^2}{D_s} u_s = 0, \qquad 1 < z < \frac{x_w + (x_s - x_s)}{x_s}, \qquad 0 < \tau < 1$$

$$\Rightarrow \frac{d^2 u_s}{dz^2} - \underbrace{\frac{kx_s^2}{D_s}}_{\gamma} u_s = 0, \qquad 1 < z < 1 + \underbrace{\frac{x_w - x_s}{x_s}}_{w}, \qquad 0 < \tau < 1$$

Rescaling

The initial condition becomes:

$$
\begin{gathered}
u_g C_0 = C_0, \quad 0 < zx_s < x_s, \quad \tau L = 0 \\
\Rightarrow \quad u_g = 1, \quad 0 < z < 1, \quad \tau = 0 \\
\Rightarrow u_g(z,0) = 1, \quad z \in (0,1)
\end{gathered}
$$

The boundary conditions becomes:

$$
\begin{gathered}
\frac{\partial(u_g C_0)}{\partial(zx_s)} = 0, \quad zx_s = 0, \quad 0 < \tau L < L \Rightarrow \frac{C_0}{x_s}\frac{\partial u_g}{\partial z} = 0, \quad z = 0, \quad 0 < \tau < 1 \\
\frac{\partial u_g}{\partial z}(0,\tau) = 0, \quad \tau \in (0,1)
\end{gathered}
$$

$$
\begin{gathered}
\frac{d(u_s C_0)}{d(zx_s)} = 0, \quad zx_s = x_w, \quad 0 < \tau L < L \Rightarrow \frac{C_0}{x_s}\frac{du_s}{dz} = 0, \quad z = 1 + w, \quad 0 < \tau < 1 \\
\frac{du_s}{dz}(1+w,\tau) = 0, \quad \tau \in (0,1)
\end{gathered}
$$

Rescaling

The interface conditions becomes:

$$u_g C_0 = u_s C_0, \quad zx_s = x_s, \quad 0 < \tau L < L \Rightarrow u_g = u_s, \quad z = 1, \quad 0 < \tau < 1$$
$$\Rightarrow u_g(1,\tau) = u_s(1,\tau), \quad \tau \in (0,1)$$

$$D_g \frac{\partial(u_g C_0)}{\partial(zx_s)} = D_s \frac{d(u_s C_0)}{d(zx_s)}, \quad zx_s = x_s, \quad 0 < \tau L < L$$
$$\Rightarrow D_g \frac{C_0}{x_s}\frac{\partial u_g}{\partial z} = D_s \frac{C_0}{x_s}\frac{du_s}{dz}, \quad z = 1, \quad 0 < \tau < 1$$
$$\Rightarrow \frac{\partial u_g}{\partial z}(1,\tau) = \underbrace{\frac{D_s}{D_g}}_{\alpha} \frac{du_s}{dz}(1,\tau), \quad \tau \in (0,1)$$

Rescaling

In summary, we consider this problem from here on out:

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

$$\textbf{ODE:}\ \frac{d^2 u_s}{dz^2}(z,\tau) - \gamma u_s(z,\tau) = 0, \quad z \in (1, 1+w), \quad \tau \in (0,1)$$

$$\textbf{Initial Condition:}\ u_g(z,0) = 1, \quad z \in (0,1)$$

$$\textbf{Boundary Conditions:}\ \frac{\partial u_g}{\partial z}(0,\tau) = \frac{du_s}{dz}(1+w,\tau) = 0, \quad \tau \in (0,1)$$

$$\textbf{Interface Conditions:}\ u_g(1,\tau) = u_s(1,\tau), \quad \frac{\partial u_g}{\partial z}(1,\tau) = \alpha\frac{du_s}{dz}(1,\tau), \quad \tau \in (0,1)$$

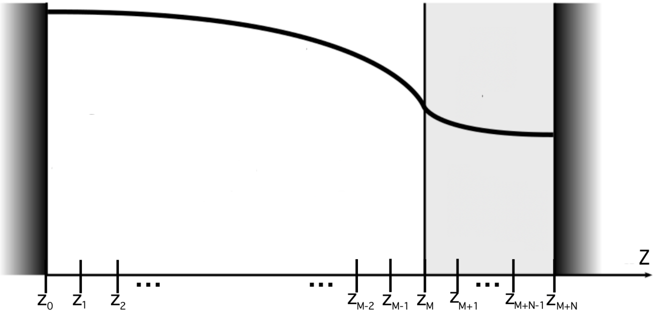
Where the variables $v(z), \eta, \gamma, w, \alpha$ are defined as:

$$v(z) = \left(1 - 4\left[z - \frac{1}{2}\right]^2\right), \quad \eta = \frac{D_g L}{V_{max} x_s^2}, \quad \gamma = \frac{k x_s^2}{D_s}$$

$$w = \frac{x_w - x_s}{x_s}, \quad \alpha = \frac{D_s}{D_g}$$

Discretization

A uniform discretization is made for this new rescaled problem, $z_j = j\Delta z$, where $z_M = 1$ and $z_{M+N} = 1 + w$.
We introduce the notations:
$u_g^j(\tau) \approx u_g(z_j, \tau)$,
$u_s^j(\tau) \approx u_s(z_{M+j}, \tau)$ and
$u_g(1, \tau) = u_s(1, \tau) = \bar{u}$



Discretization

- 2:nd order finite difference approximation for the inner grid points (central difference)
- 2:nd order for outer boundaries (Skewed approximation for the Neumann conditions)
- For interface conditions: 1:st order finite difference approximation (backwards/forwards difference)

Discretization

Leads to the following system of equations:

- 1) PDE:

$$\frac{\partial u_g}{\partial \tau}(z_j,\tau) = \frac{\eta}{v(z_j)} \frac{u_g^{j+1}(\tau) - 2u_g^j(\tau) + u_g^{j-1}(\tau)}{\Delta z^2}$$

- 2) ODE:

$$\frac{u_s^{j+1}(\tau) - 2u_s^j(\tau) + u_s^{j-1}(\tau)}{\Delta z^2} - \gamma u_s^j(\tau) = 0$$

Discretization

Using the Neumann boundary conditions, together with skewed FD approximation:

- First row of PDE:

$$\Rightarrow \frac{\eta}{v(z_1)} \frac{2u_g^2(\tau) - 2u_g^1(\tau)}{3\Delta z^2} = 0$$

- Last row of ODE:

$$\Rightarrow \frac{2u_s^{N-2}(\tau) - 2u_s^{N-1}(\tau)}{3\Delta z^2} - \gamma u_s^{N-1}(\tau) = 0$$

Discretization

Moreover, for the interface conditions: $u_g(1,\tau) = u_s(1,\tau)$, $\frac{\partial u_g}{\partial z}(1,\tau) = \alpha \frac{\partial u_s}{\partial z}(1,\tau)$:

- The following equation is constructed:

$$\begin{aligned}
\frac{\partial u_g}{\partial z}(1,\tau) &= \alpha \frac{\partial u_s}{\partial z}(1,\tau) \\
\Rightarrow \frac{u_g^M(\tau) - u_g^{M-1}(\tau)}{\Delta z} - \alpha \frac{u_s^1(\tau) - u_s^0(\tau)}{\Delta z} &= 0 \\
\Rightarrow \frac{\bar{u}(\tau) - u_g^{M-1}(\tau)}{\Delta z} - \alpha \frac{u_s^1(\tau) - \bar{u}(\tau)}{\Delta z} &= 0
\end{aligned}$$

Discretization

- Equations from previous slides eventually lead to the following block matrix system, consisting of $A_1 \in \mathbb{R}^{(M-1)\times(M-1)}$, $\boldsymbol{e}_1 \in \mathbb{R}^{M-1}$, $0_1 \in \mathbb{R}^{(M-1)\times(N-1)}$, $\boldsymbol{b}_1^T \in \mathbb{R}^{1\times(M-1)}$, $a \in \mathbb{R}$, $\boldsymbol{b}_2^T \in \mathbb{R}^{1\times(N-1)}$, $0_2 \in \mathbb{R}^{(N-1)\times(M-1)}$, $\boldsymbol{e}_2 \in \mathbb{R}^{N-1}$, $A_2 \in \mathbb{R}^{(N-1)\times(N-1)}$:

$$
\begin{matrix}
\begin{bmatrix}
\frac{-2\eta}{3v(z_1)\Delta z^2} & \frac{2\eta}{3v(z_1)\Delta z^2} & \cdots & \\
\frac{\eta}{v(z_2)\Delta z^2} & \frac{-2\eta}{v(z_2)\Delta z^2} & \frac{\eta}{v(z_2)\Delta z^2} & \\
\vdots & \ddots & & \\
 & & \frac{\eta}{v(z_{M-1})\Delta z^2} & \frac{-2\eta}{v(z_{M-1})\Delta z^2}
\end{bmatrix}
&
\begin{bmatrix}
0 \\ \vdots \\ \frac{\eta}{v(z_{M-1})\Delta z^2}
\end{bmatrix}
&
\begin{bmatrix}
0 & \cdots & 0 \\
\vdots & & \vdots \\
0 & \cdots & 0
\end{bmatrix}
\\
\begin{bmatrix}
0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \frac{-1}{\Delta z}
\end{bmatrix}
&
\begin{bmatrix}
\frac{1+\alpha}{\Delta z}
\end{bmatrix}
&
\begin{bmatrix}
\frac{-\alpha}{\Delta z} & \cdots & 0
\end{bmatrix}
\\
\begin{bmatrix}
0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
\vdots & & & & & & & \vdots \\
0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0
\end{bmatrix}
&
\begin{bmatrix}
\frac{1}{\Delta z^2} \\ \vdots \\ 0
\end{bmatrix}
&
\begin{bmatrix}
\frac{-2}{\Delta z^2} - \gamma & \frac{1}{\Delta z^2} & \cdots \\
\ddots & & \\
 & \frac{2}{3\Delta z^2} & \frac{-2}{3\Delta z^2} - \gamma
\end{bmatrix}
\end{matrix}
$$

Discretization

We get the following DAE system to be solved:

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

Implicit Euler

The Implicit Euler method for the system is formulated as

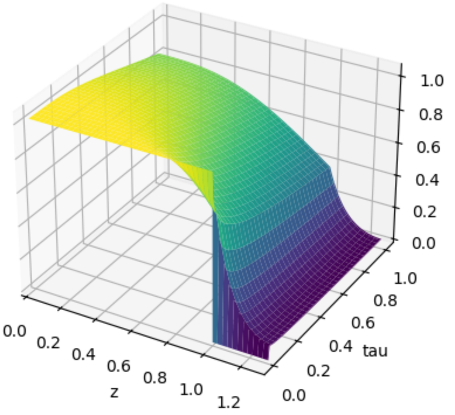
$$\begin{pmatrix} \mathbf{u}_g^{n+1} \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \mathbf{u}_g^{n} \\ 0 \\ 0 \end{pmatrix} + \Delta\tau \underbrace{\begin{pmatrix} A_1 & \mathbf{e}_1 & 0 \\ \mathbf{b}_1^T & a & \mathbf{b}_2^T \\ 0 & \mathbf{e}_2 & A_2 \end{pmatrix}}_{A} \begin{pmatrix} \mathbf{u}_g^{n+1}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

Reduced to $B\boldsymbol{u}_g^{n+1} = \begin{pmatrix} \boldsymbol{u}_g^{n} \\ 0 \\ 0 \end{pmatrix}$

where

$$B = \left[\begin{pmatrix} I_{M-1,M-1} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \Delta\tau A \right]$$

eta=0.2 gamma=100 alpha=0.2 w=0.3 epsilon=0



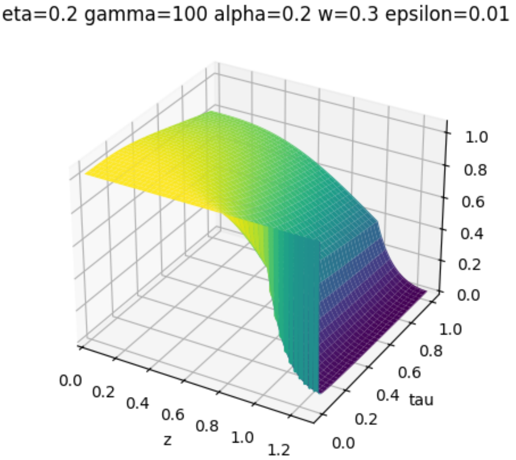
Implicit Euler. $\boldsymbol{u}_0 = [\mathbf{1}, 0, \mathbf{0}]^T$

Regularization with Implicit Euler

The system can be turned into a ODE system of the form:

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

by adding a regularization parameter $0 < \epsilon \ll 1$
The ODE is then solved with Implicit Euler



Regularization and impl. Euler. $\boldsymbol{u}_0 = [\mathbf{1}, 1, \mathbf{1}]^T$

Analytic Reduction + Implicit Euler

The PDE+ODE system can be reduced to just a PDE by finding an analytical solution, $u_s(z,\tau)$
Start with a general linear solution:

$$u_s(z,\tau) = c_1(\tau)e^{z\sqrt{\gamma}} + c_2(\tau)e^{-z\sqrt{\gamma}}$$

Use boundary condition, $\frac{\partial u_s}{\partial z}(1+w,\tau) = 0$, to find expression for $c_1(\tau)$

$$\frac{\partial u_s}{\partial z}(z,\tau) = \sqrt{\gamma}c_1(\tau)e^{z\sqrt{\gamma}} - \sqrt{\gamma}c_2(\tau)e^{-z\sqrt{\gamma}} \Rightarrow$$

$$\frac{\partial u_s}{\partial z}(1+w,\tau) = \sqrt{\gamma}c_1(\tau)e^{(1+w)\sqrt{\gamma}} - \sqrt{\gamma}c_2(\tau)e^{-(1+w)\sqrt{\gamma}} = 0 \Rightarrow$$

$$\Rightarrow c_1(\tau) = \frac{c_2(\tau)}{e^{2(1+w)\sqrt{\gamma}}}$$

Which gives u_s as:

$$u_s(z,\tau) = \frac{c_2(\tau)}{e^{2(1+w)\sqrt{\gamma}}}e^{z\sqrt{\gamma}} + c_2(\tau)e^{-z\sqrt{\gamma}}$$

Analytic Reduction + Implicit Euler

Next we can use the interface conditions, $u_g(1,\tau) = u_s(1,\tau)$ and $\frac{\partial u_g}{\partial z}(1,\tau) = \alpha \frac{\partial u_s}{\partial z}(1,\tau)$ to get expressions for $u_g(1,\tau)$ and $\frac{\partial u_g}{\partial z}(1,\tau)$:

$$u_g(1,\tau) = \frac{c_2(\tau)}{e^{2(1+w)\sqrt{\gamma}}} e^{\sqrt{\gamma}} + c_2(\tau) e^{-\sqrt{\gamma}}$$

$$\frac{\partial u_g}{\partial z}(1,\tau) = \alpha \left(\sqrt{\gamma} \frac{c_2(\tau)}{e^{2(1+w)\sqrt{\gamma}}} e^{\sqrt{\gamma}} - \sqrt{\gamma} c_2(\tau) e^{-\sqrt{\gamma}} \right)$$

for simplicity we can describe the boundary using this equation:

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

where:

$$\beta = \alpha\sqrt{\gamma} \left(\frac{1 - \frac{1}{e^{(2w\sqrt{\gamma})}}}{\frac{1}{e^{(2w\sqrt{\gamma})}} + 1} \right) = \alpha\sqrt{\gamma}\tanh(w\sqrt{\gamma})$$

Analytic Reduction + Implicit Euler

Instead of the PDE+ODE problem before we now have changed the boundary condition of the PDE to take into account the absorption of gas. The problem:

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

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

The new boundary can be discretized with a skewed difference approximation:

$$\frac{du_g}{dz}(1,\tau) + \beta u_g(1,\tau) = 0 \Rightarrow \frac{3u_g(1,\tau) - 4u_g(1-\Delta z,\tau) + u_g(1-2\Delta z,\tau)}{2\Delta z} + \beta u_g(1,\tau) = 0$$

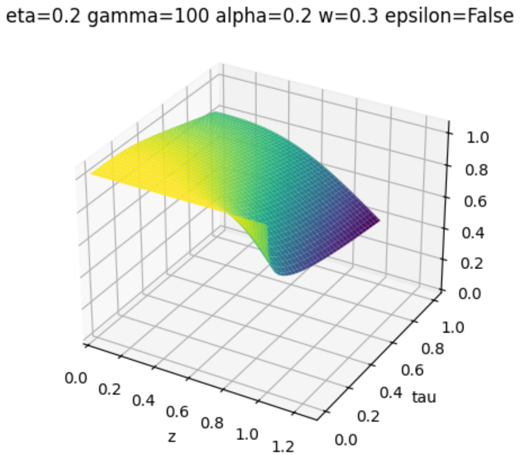
which changes the last row in the "A1" matrix from before into:

$$\left(\frac{\eta}{v(z_{M-1})\Delta z^2}\frac{-2-4\Delta z\beta}{3+2\Delta z\beta}\right)u_g^{M-1} + \left(\frac{\eta}{v(z_{M-1})\Delta z^2}\frac{2+2\Delta z\beta}{3+2\Delta z\beta}\right)u_g^{M-2}$$

Analytic Reduction + Implicit Euler

- We get the equation system: $\frac{d\mathbf{u}_g}{d\tau} = A_1 \mathbf{u}_g$
- Solving this system is done with implicit Euler:

$$\mathbf{u}_g^{n+1} = \mathbf{u}_g^n + \Delta\tau A_1 \mathbf{u}_g^{n+1}$$
$$\Rightarrow$$
$$\underbrace{[I - \Delta\tau A_1]}_{B} \mathbf{u}_g^{n+1} = \mathbf{u}_g^n$$



Note that the ODE $(1 < z \leq 1 + w)$ part is not in this solution.

Numerical Investigation Results

All three methods yields very similar result for M=1000 and $\Delta\tau = \frac{1}{1000}$

- Implicit Euler
  - \+ Robust (always stable, regardless of $\Delta\tau$ size)
  - \- Slower than Analytic Reduction + Implicit Euler
- Regularization + Implicit Euler
  - \+ Replaces algebraic constraints with ODE
  - \- Has to choose the right size of ϵ
  - \- Not as accurate
- Analytic Reduction + Implicit Euler
  - \+ Smaller system to solve
  - \+ Quicker (Because of size)
  - \- More work "by hand"

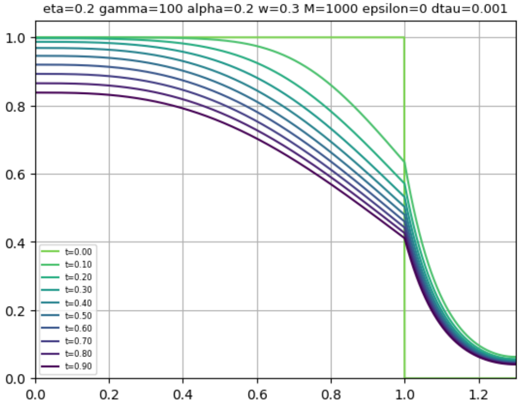
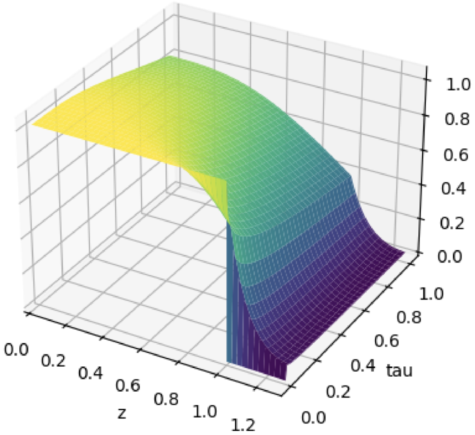


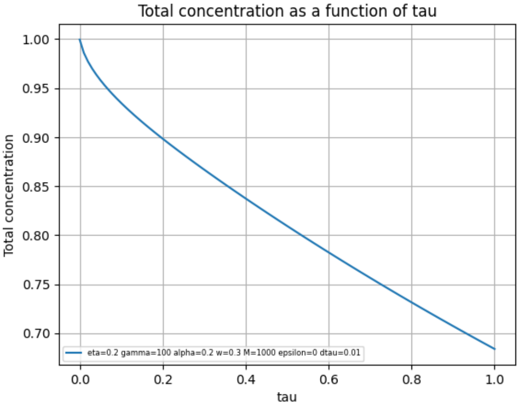
Figure: Implicit Euler for different τ, starting with $\mathbf{u}_g = \mathbf{1}, \bar{u} = 0, \mathbf{u}_s = \mathbf{0}$

Investigations of the solution

Integrating the solution over the z domain gives the total concentration in a cross section of the pipe. Shows how the catalytic reaction removes the unwanted compound.

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





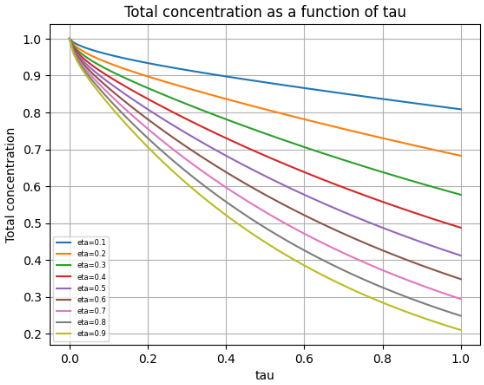
Investigations of the solution

We can now investigate how the physical properties of the initial problem affect the solution when constants are changed.

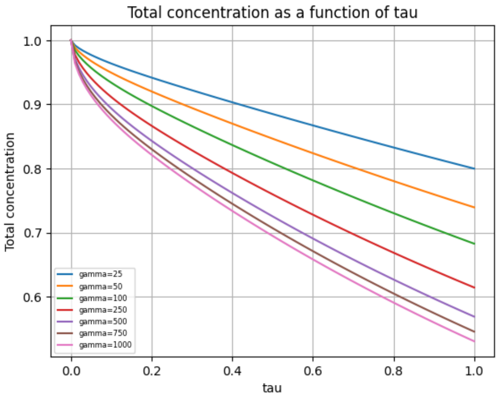
- Recall the dimensionless constants:

$$w = \frac{x_w - x_s}{x_s}, \quad \alpha = \frac{D_s}{D_g}, \quad \eta = \frac{D_g L}{V_{\max} x_s^2}, \quad \gamma = \frac{k x_s^2}{D_s}$$

- Varying $\eta = \frac{D_g L}{V_{\max} x_s^2}$

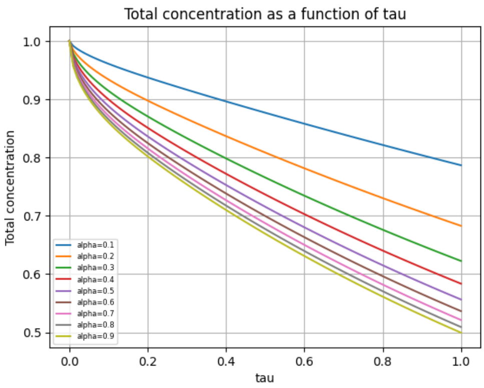


- Varying $\gamma = \frac{k x_s^2}{D_s}$

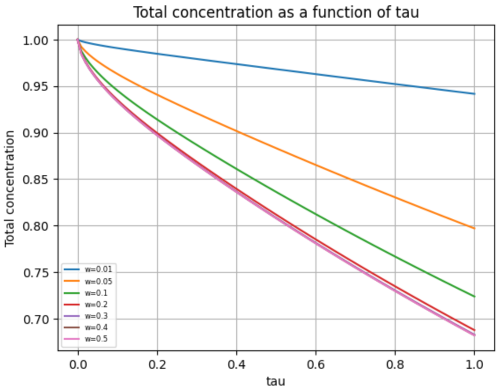


Investigations of the solution

- Varying $\alpha = \frac{D_s}{D_g}$



- Varying $w = \frac{x_w - x_s}{x_s}$



Investigations of the solution

Summary

- Want γ large $\rightarrow$ x_s large gives by Bernoulli's principle $\rightarrow$ V_{max} small
- Want η large $\rightarrow$ Large L and D_g
- Want α sufficiently high $\rightarrow$ D_s close to D_g
- Want the catalyst to be sufficiently wide
- By increasing constants w and γ we increase β since $\beta = \alpha\sqrt{\gamma}\tanh(w\sqrt{\gamma})$

QUESTIONS?