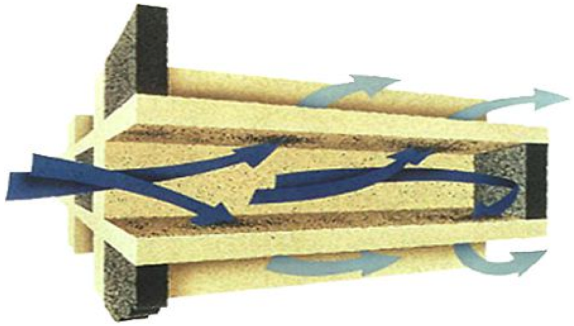
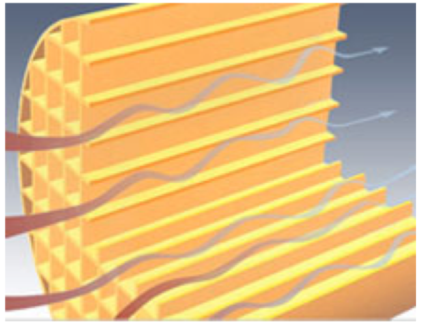
2.29 Class Project | Thursday, May 16th

Solving Stiff Problems in Flow Thorough Catalysts

Flow through catalysts

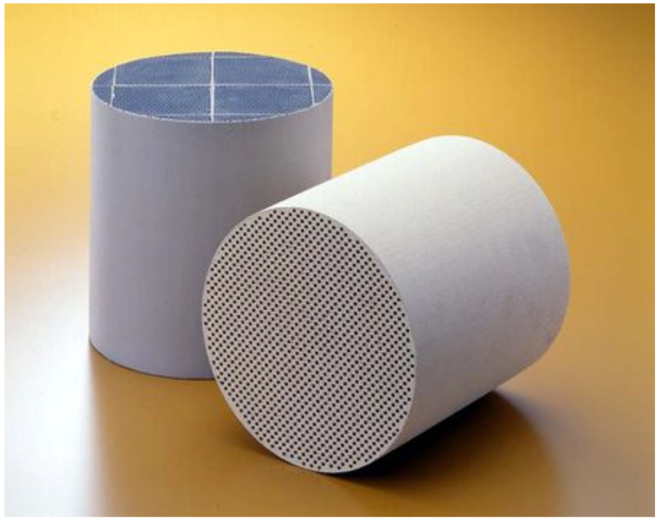




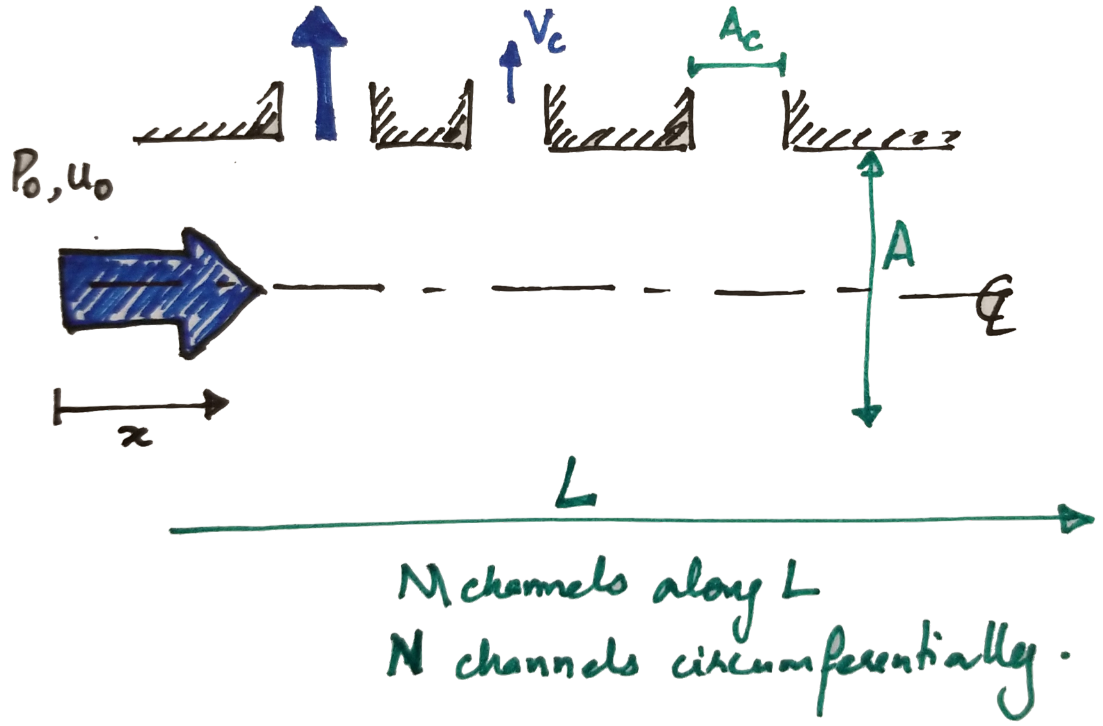
Selective Catalytic Reduction reduces NO_x emissions in diesel engines by 98%

Important to understand the flow in the catalyst to be able to:

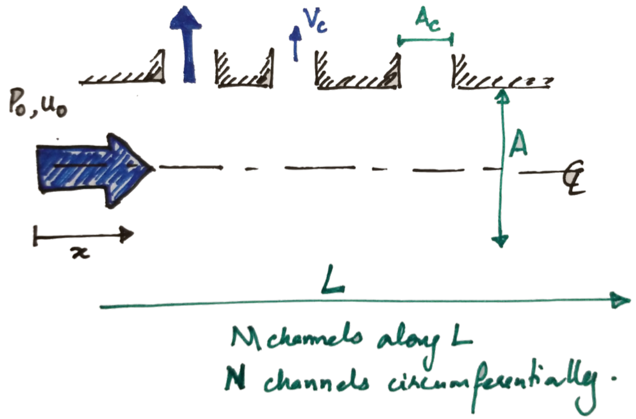
- estimate the performance of the catalyst
- estimate the pressure drop induced by the catalyst



Simplified problem – “perforated pipe problem”



Derivation of equations



- Mass Conservation

$$v_c = \frac{-AL}{A_c N M}\frac{du}{dx}$$

- Momentum

$$\frac{1}{\rho}\frac{dP}{dx} + \frac{f_D}{2D_h}u^2\left(1 - \frac{a_c M}{L}\right) + u\frac{du}{dx}(2-\beta) = 0$$

- Reacting channels

$$P(x) - P_{amb} = \frac{1}{2}\rho\xi v_c^2$$

$$P(x) - P_{amb} = \frac{1}{2}\rho\xi\left(\frac{AL}{A_c N M}\right)^2\left(\frac{du}{dx}\right)^2$$

Set-up governing equation

$$U = \frac{u}{u_0}$$

$$X = \frac{x}{L}$$

$$\bar{A} = \frac{A_c N M}{A}$$

$$B = \frac{2-\beta}{\xi}$$

$$F = \frac{f_D L}{2 D_h \xi}$$

$$\bar{L} = 1 - \frac{a_c M}{L}$$

$$\xi \frac{AL}{A_c N M} \frac{du}{dx} \frac{d^2 u}{dx^2} + \frac{f_D}{2D_h} u^2 \left(1 - \frac{a_c M}{L}\right) + u \frac{du}{dx}(2-\beta) = 0$$

$$\frac{dU}{dX}\left(\frac{d^2 U}{dX^2}\right) + (B\bar{A})U\frac{dU}{dX} + (F\bar{A}\bar{L})U^2 = 0$$

Fixed Point iteration to solve the non-linear system

Non-linear solve using fixed point iteration

$$\frac{dU}{dX}\left(\frac{d^2U}{dX^2}\right) + (B\bar{A})U\frac{dU}{dX} + (F\bar{A}\bar{L})U^2 = 0$$

$$\frac{dU}{dX} = \frac{U_{i+1} - U_{i-1}}{2\Delta X} \qquad \frac{d^2U}{dX^2} = \frac{U_{i+1} - 2U_i + U_{i-1}}{(\Delta X)^2}$$

Non-linear solve using fixed point iteration

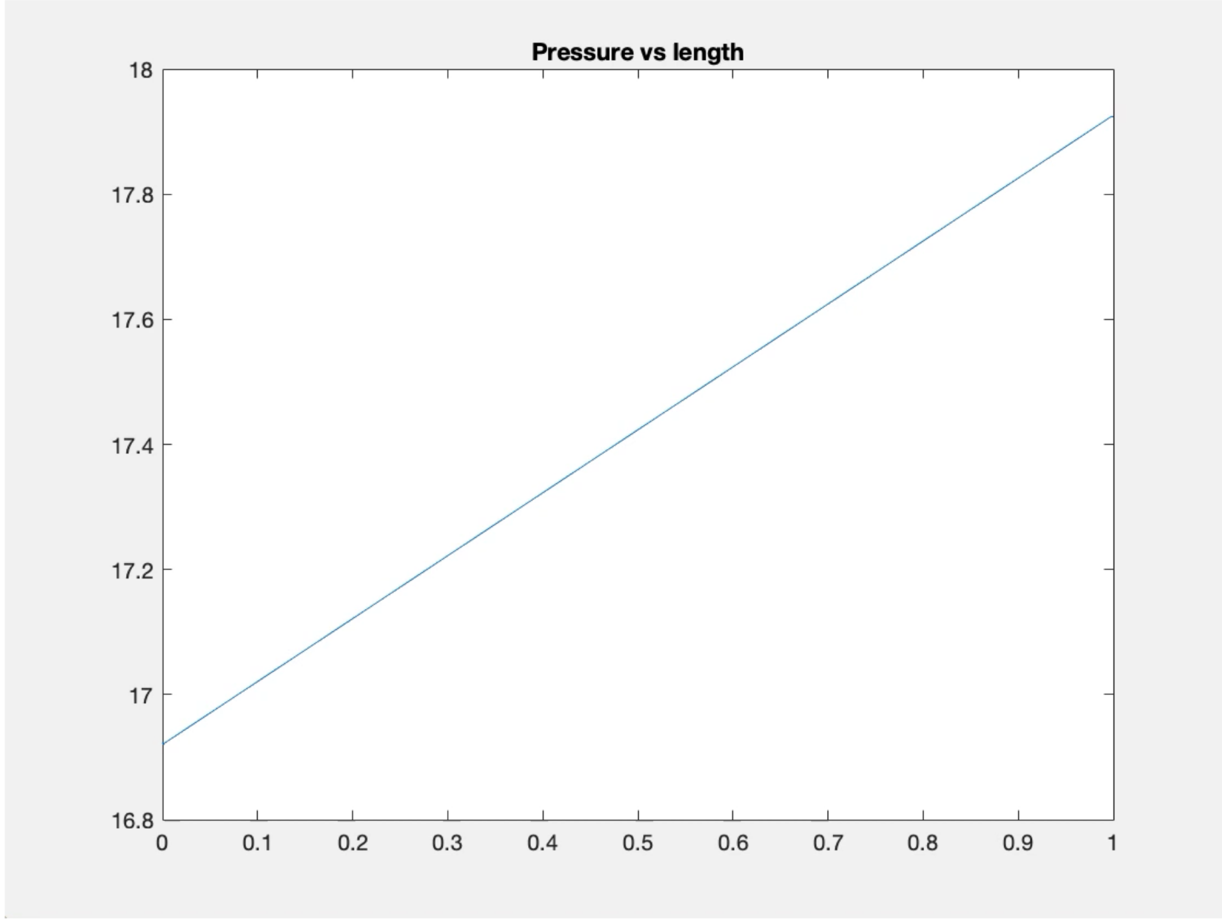
$$\frac{dU}{dX}\left(\frac{d^2U}{dX^2}\right) + (B\bar{A})U\frac{dU}{dX} + (F\bar{A}\bar{L})U^2 = 0$$

$$\vec{X} = \begin{bmatrix} U_1 \\ U_2 \\ \vdots \\ U_m \end{bmatrix} \qquad \vec{F}(X) = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_m \end{bmatrix}$$

$$\vec{G}(\vec{X}) = \vec{X} + \vec{F}(\vec{X})$$

$$\vec{G}(\vec{X}_e) = \vec{X}_e$$

BUT….


Pressure vs length
18
17.8
17.6
17.4
17.2
17
16.8
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Stiff Problem – Stiff ODE solver

*“A stiff equation is a differential equation for which certain numerical methods for solving the equation are **numerically unstable**, unless the **step size** is taken to be **extremely small**. It has proven difficult to formulate a precise definition of stiffness, but the main idea is that the equation includes **some terms** that can lead to **rapid variation in the solution**.”*

Stiff Problem – Stiff ODE solver

Commonly seen in chemistry – different reaction rates for different species involves many different time scales and this makes the problem stiff.

E.g. Global Chemistry – Transport models (GEOSChem) have very fast (~min) to very slow (~months) reactions. Packages like KPP (**Kinetic PreProcessor)** are used to solve them.

Stiff solvers use the Jacobian matrix to estimate the function behavior

ANSYS Fluent

Use a CFD package to solve – ANSYS fluent

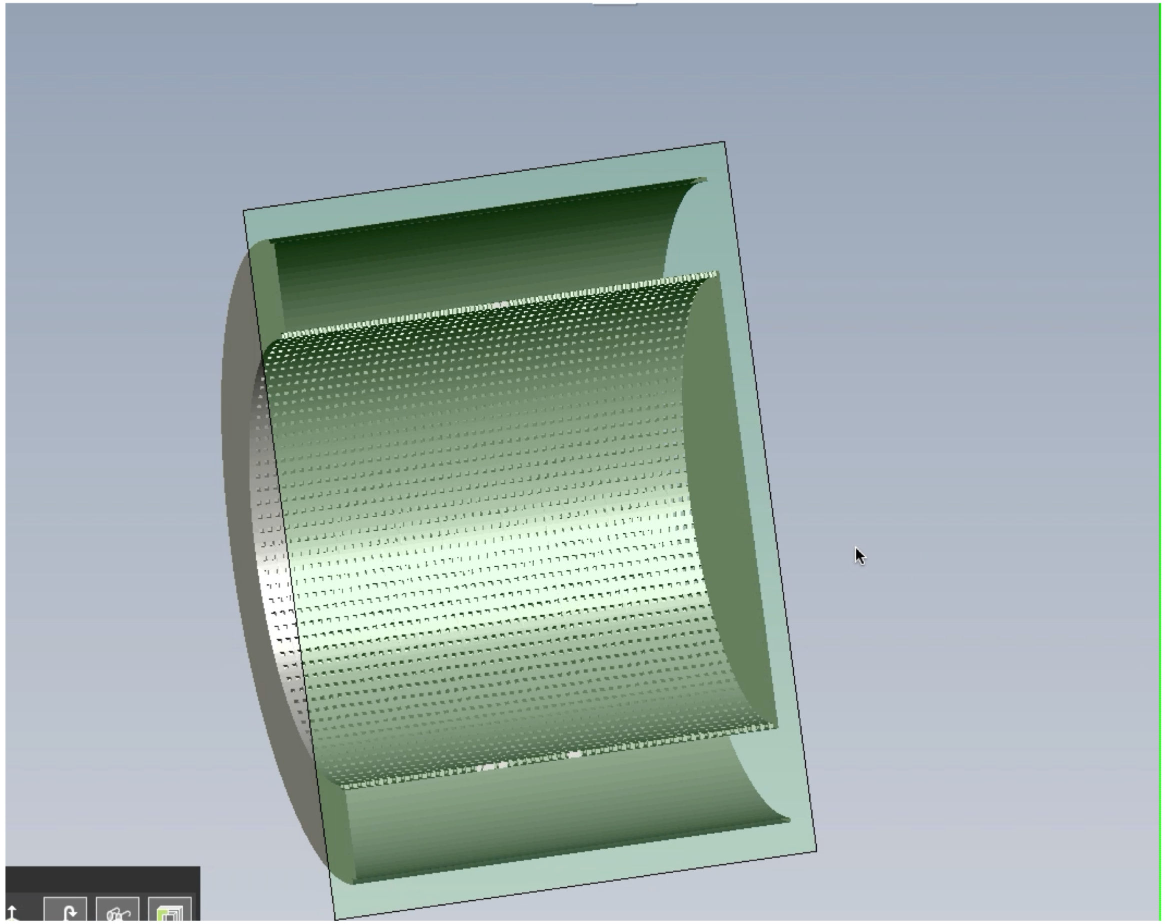
- Pressure based solver used
  - Energy Equation, S-A turbulence model

- Velocity formulation
  - Relative velocity formulation used since most of the fluid is moving

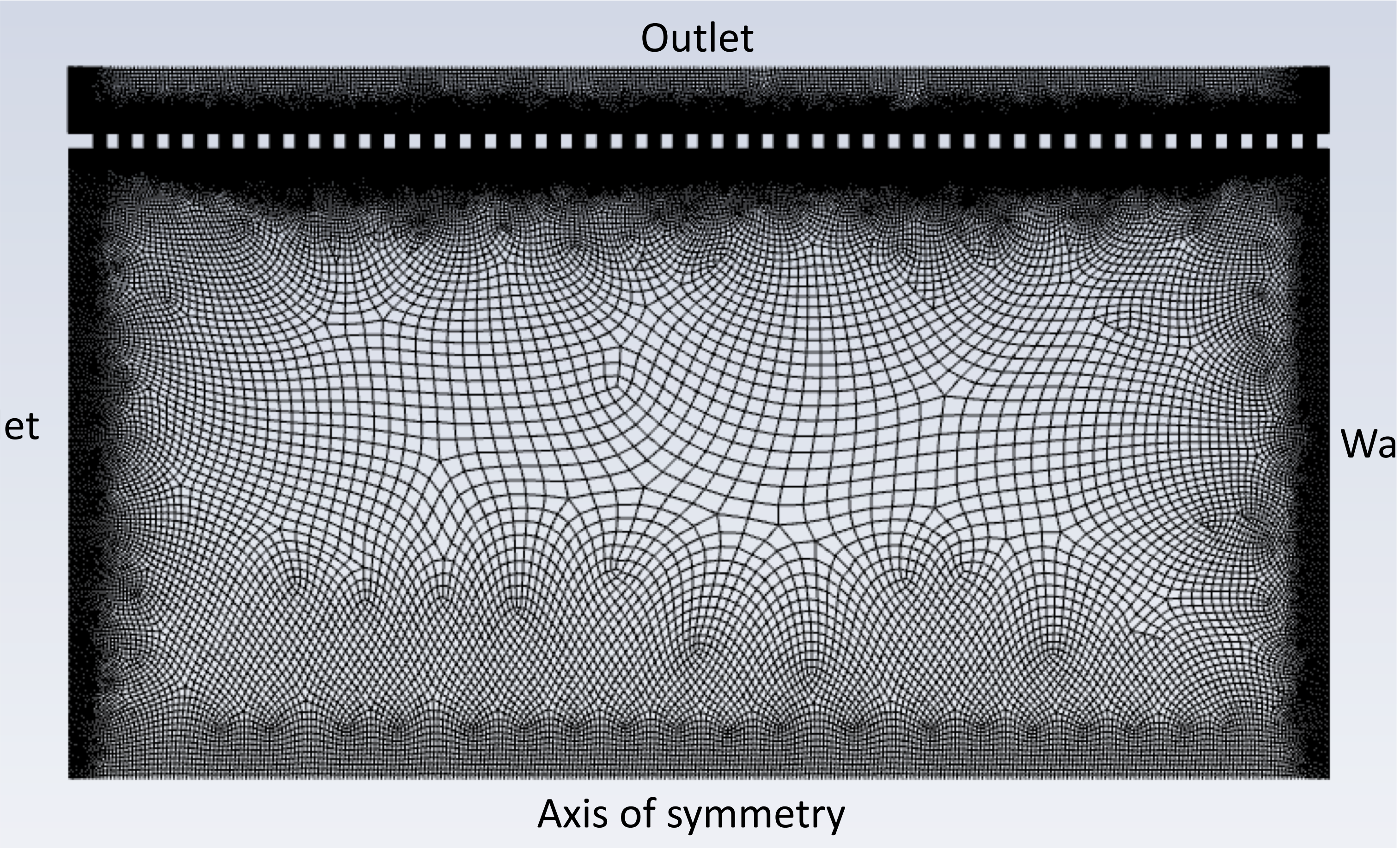
- PISO vs Coupled algorithm

  - PISO – segregated algorithm (similar to the pressure correction methods we saw in class)
  - Coupled – solves both momentum and continuity together (faster convergence)

Catalyst 3D geometry



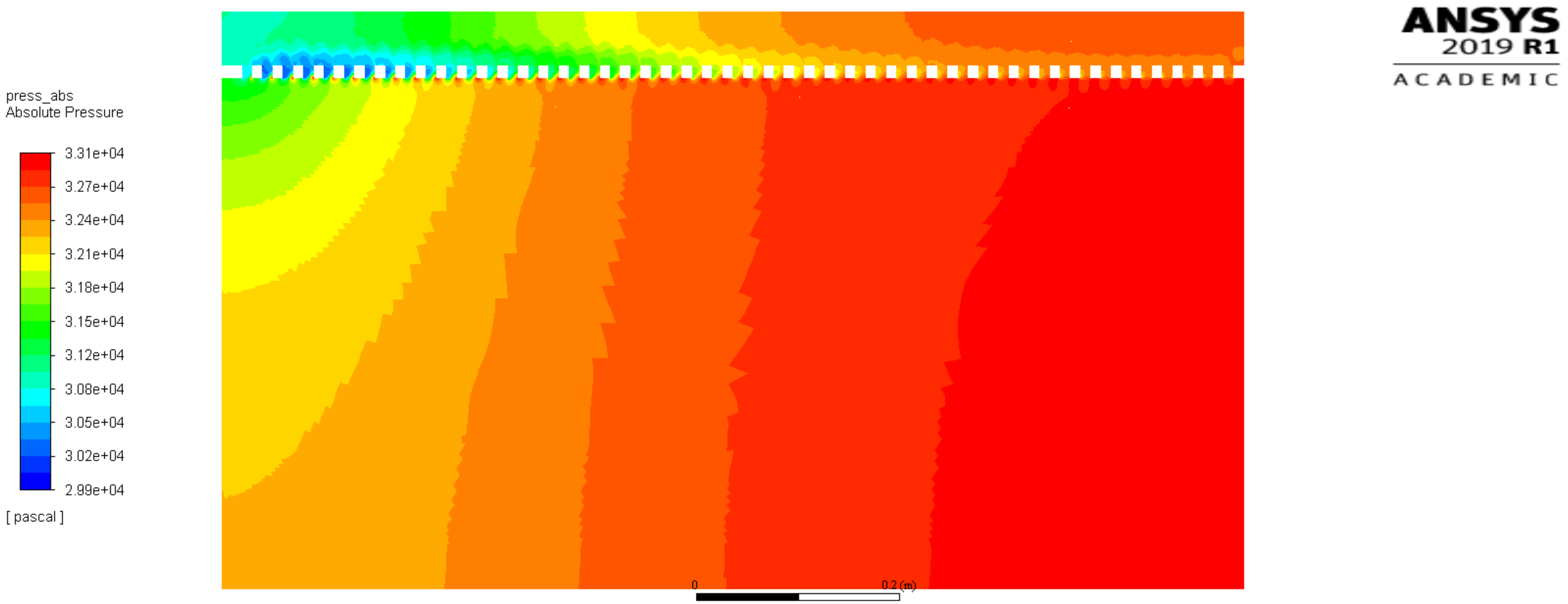
Simplified 2D geometry



0.5 Million nodes

Axisymmetric

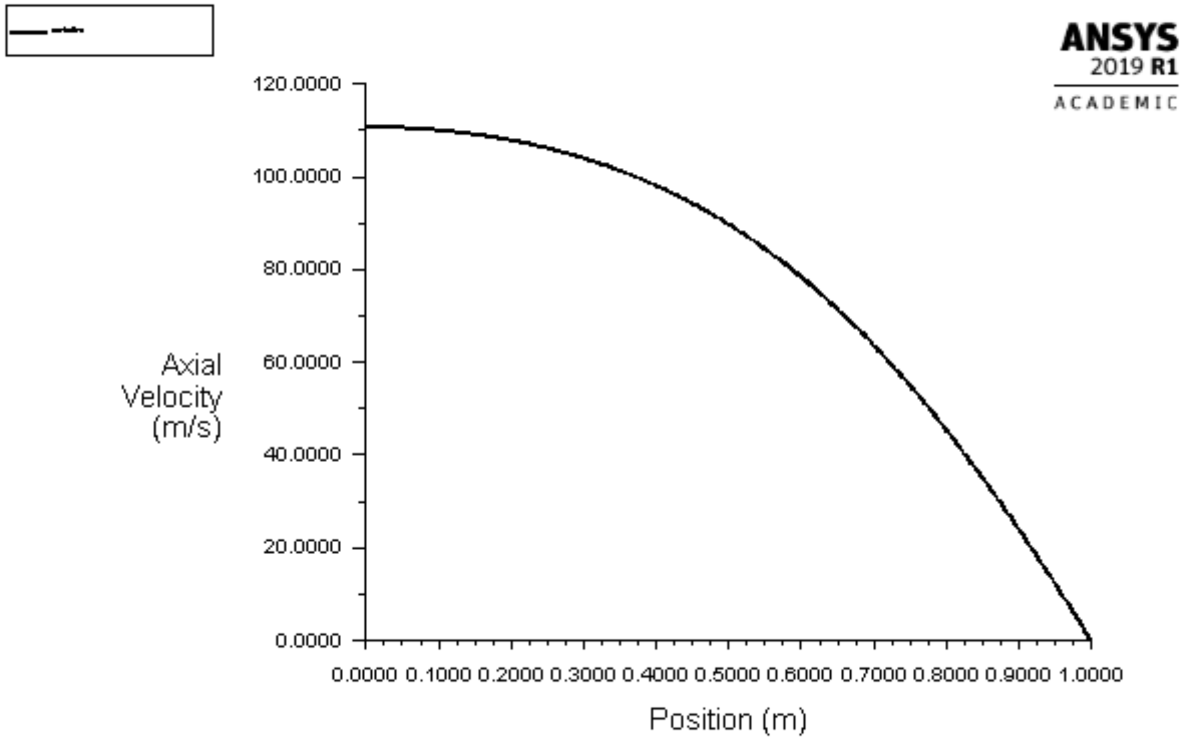
Simplified 2D geometry

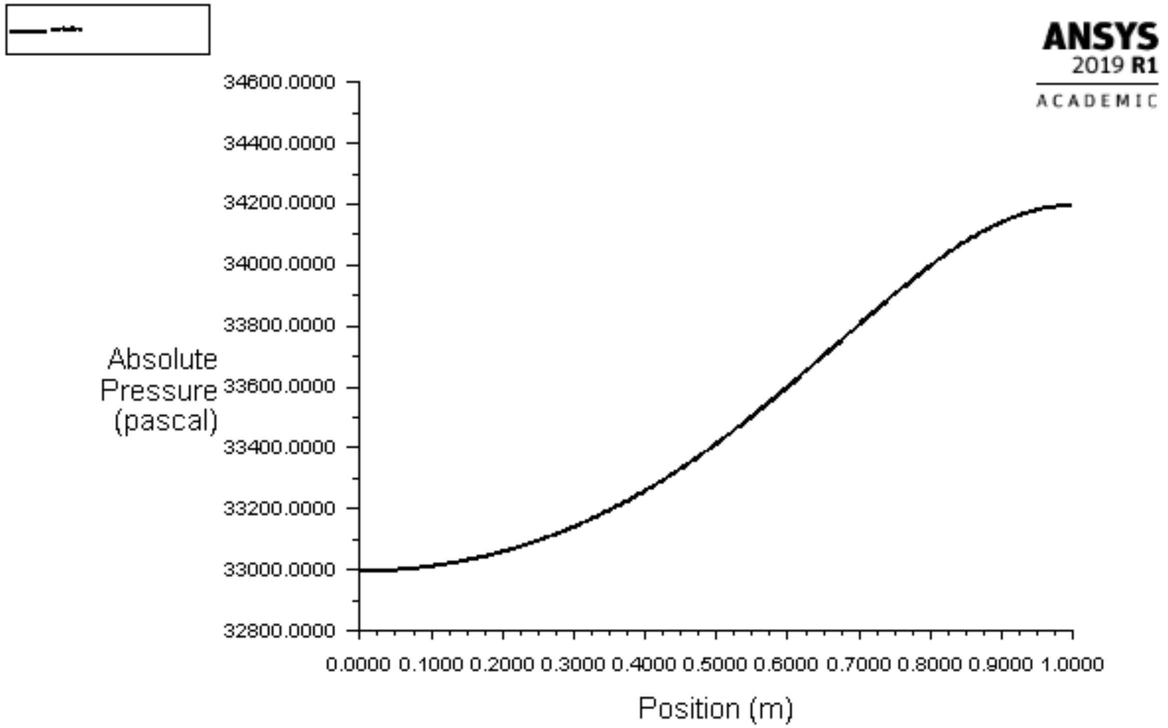


Contours of Absolute Pressure (pascal) (Time=3.0010e+00)

May 16, 2019
ANSYS Fluent 2019 R1 (axi, dp, pbns, S-A, transient)

Centerline velocity and pressure





Using a stiff solver

Solving the governing equations using a Stiff Solver

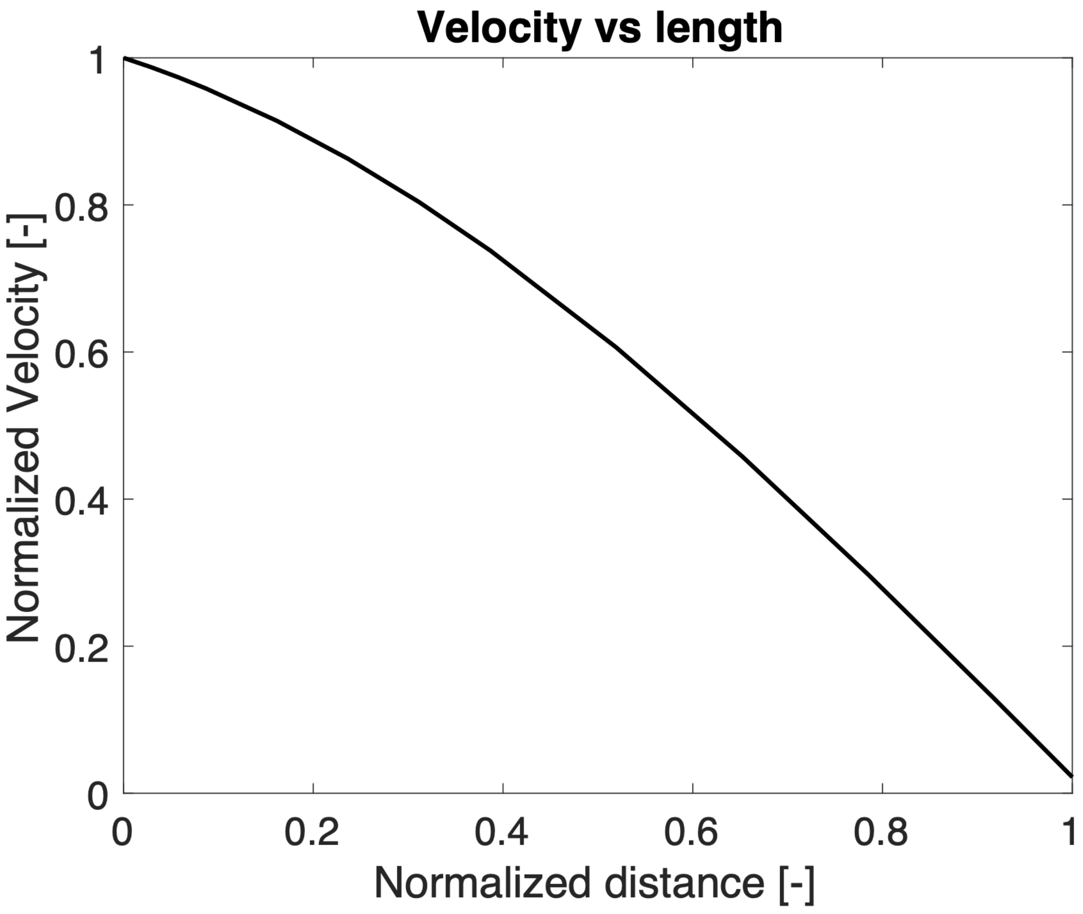
- MATLAB ode15s
- Convert eqns to system of first order ODEs

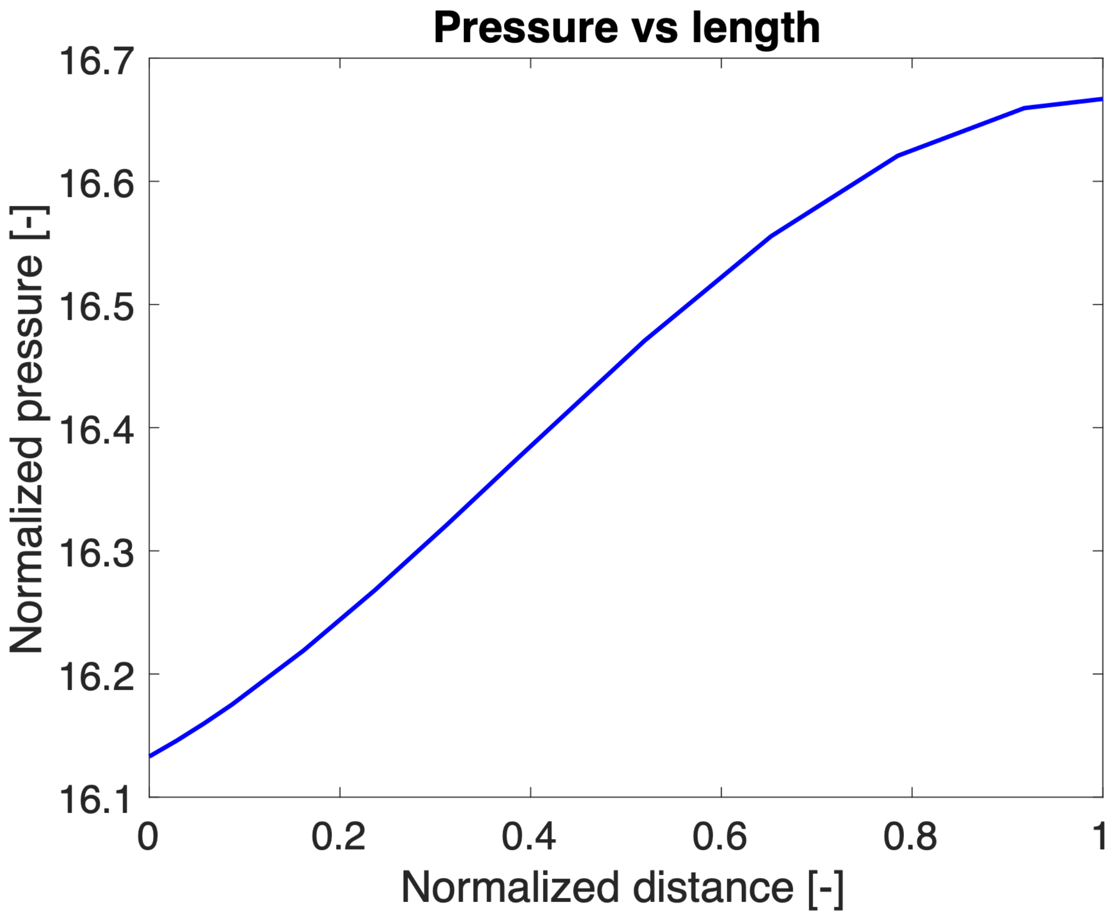
$$\frac{dU}{dX}\left(\frac{d^2U}{dX^2}\right) + (B\bar{A})U\frac{dU}{dX} + (F\bar{A}\bar{L})U^2 = 0$$

Let $y_1 = U$

$$y_1' = y_2$$
$$y_2' = -(BA)y_1 - (FAL)y_1^2/y_2$$

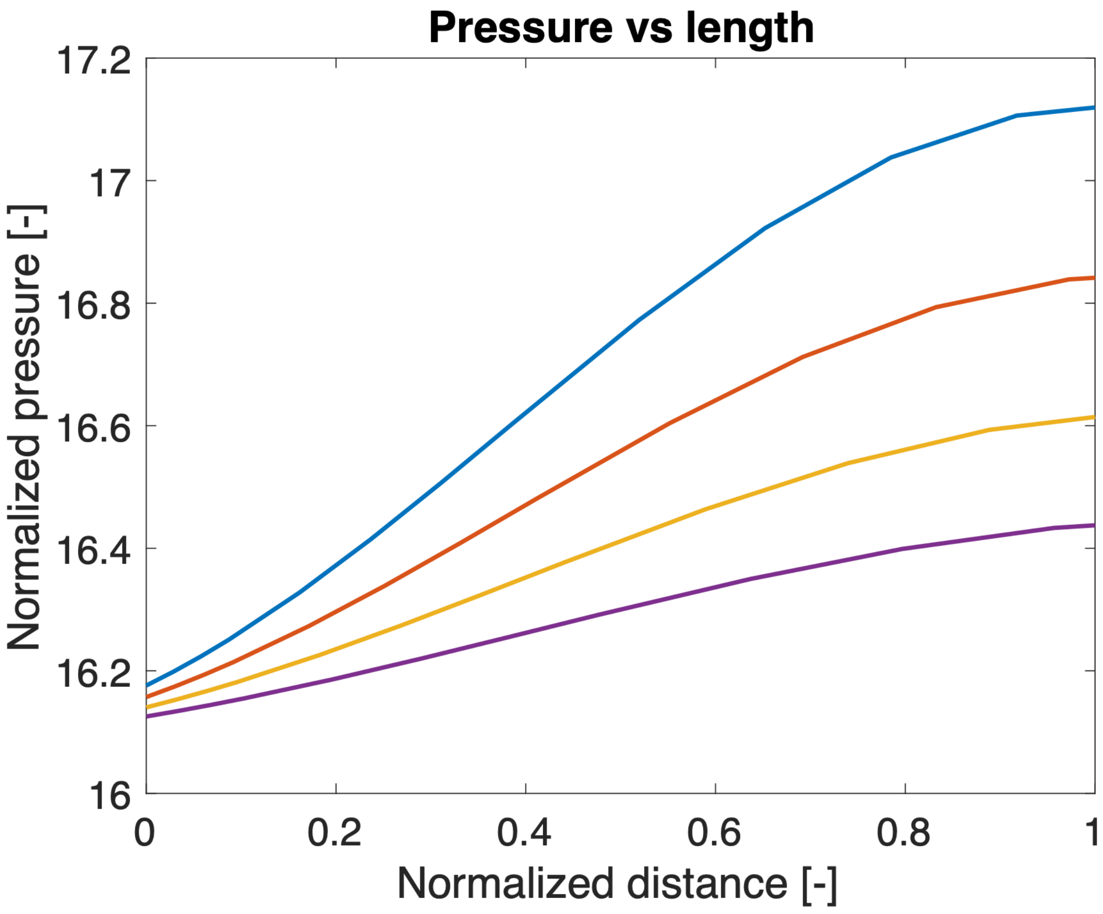
Velocity and Pressure along centerline

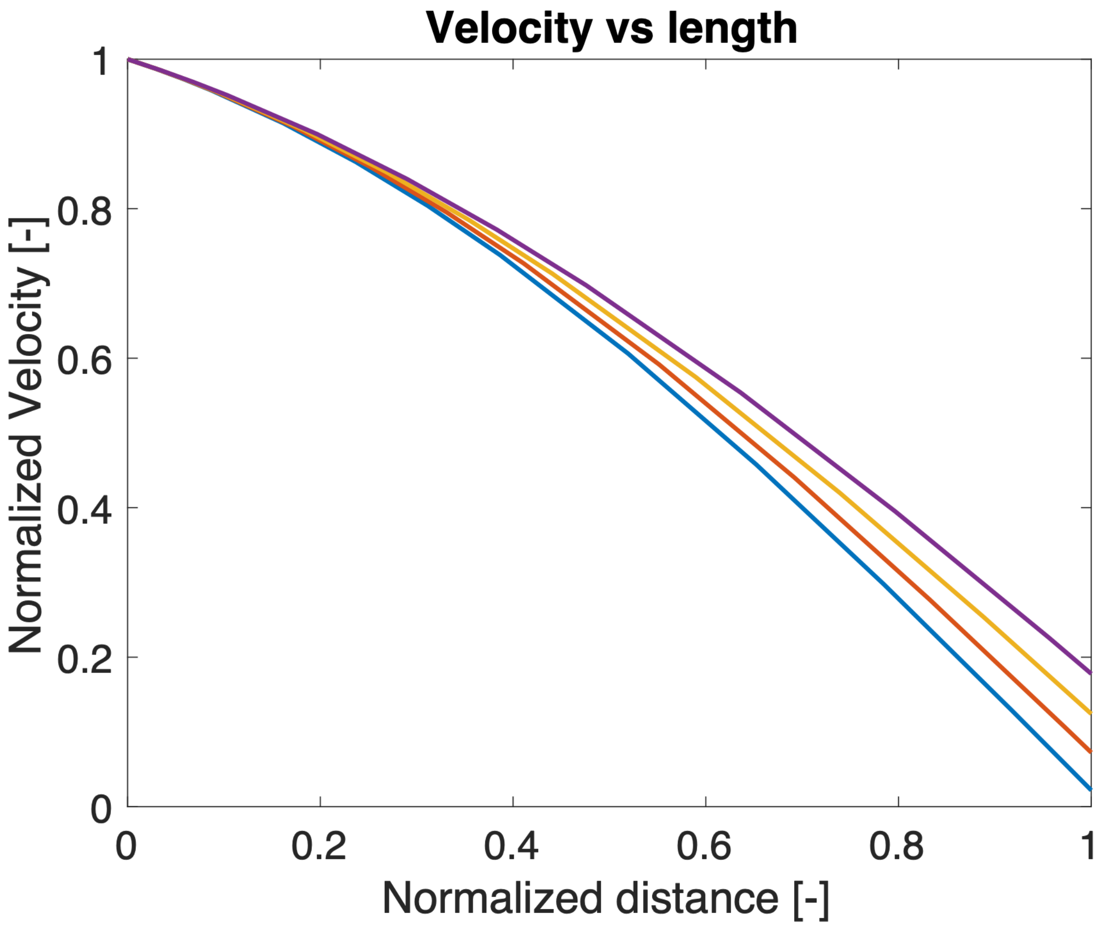




Can be used to study effects of different design choices:

E.g : Varying effective exit area





Questions