



SIMULATION AND OPTIMIZATION OF COMPRESSOR FOR CO₂ AND CO₂ - CH₄ MIXTURES IN SUPERCRITICAL CONDITIONS

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Research Centre
for Gas Innovation

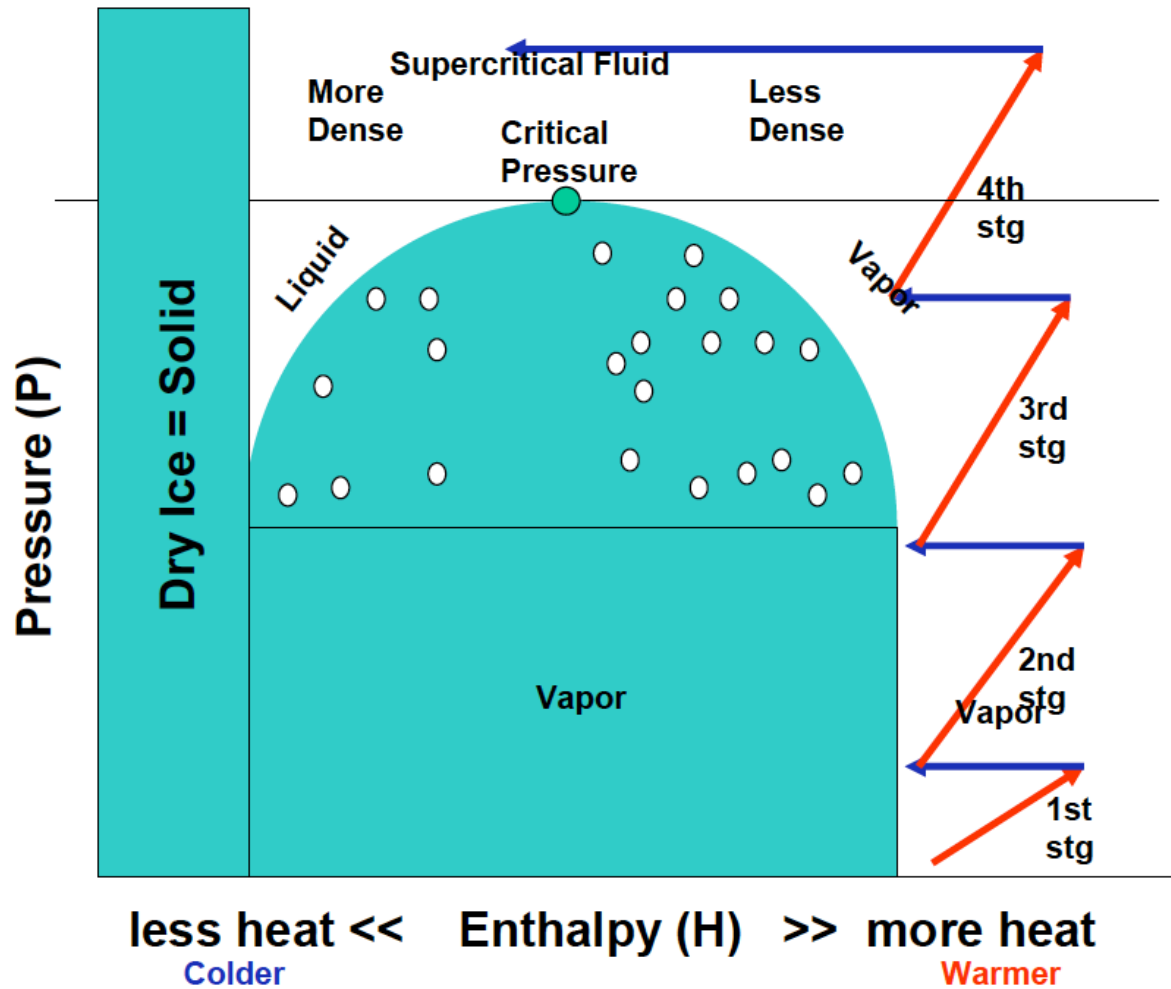
cleaner energy for a sustainable future

V Workshop Interno RCGI
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Research Team

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- **Doctoral Students:** Carlos Massaiti Okubo Junior, Luis Fernando Garcia Rodriguez
- **Master Students:** Julia Silva de Matos, Bruno Jose Nagy Antonio, Kayo Henrique Rodrigues

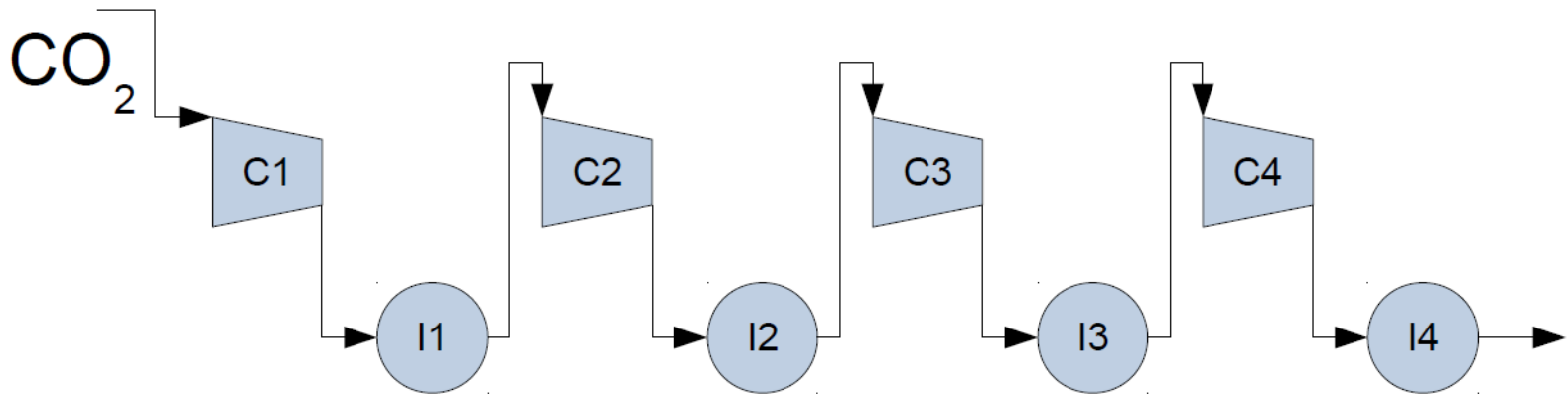
Compression of Supercritical CO2



Thermodynamic Analysis

- **Objectives**

- Estimate total power requirement as a function of the number of stages
- Determine the number of stages (actually, a decision)
- Determine inlet conditions in each stage
 - This is a requirement to proceed with rotor geometry definition and its CFD simulation for further optimization



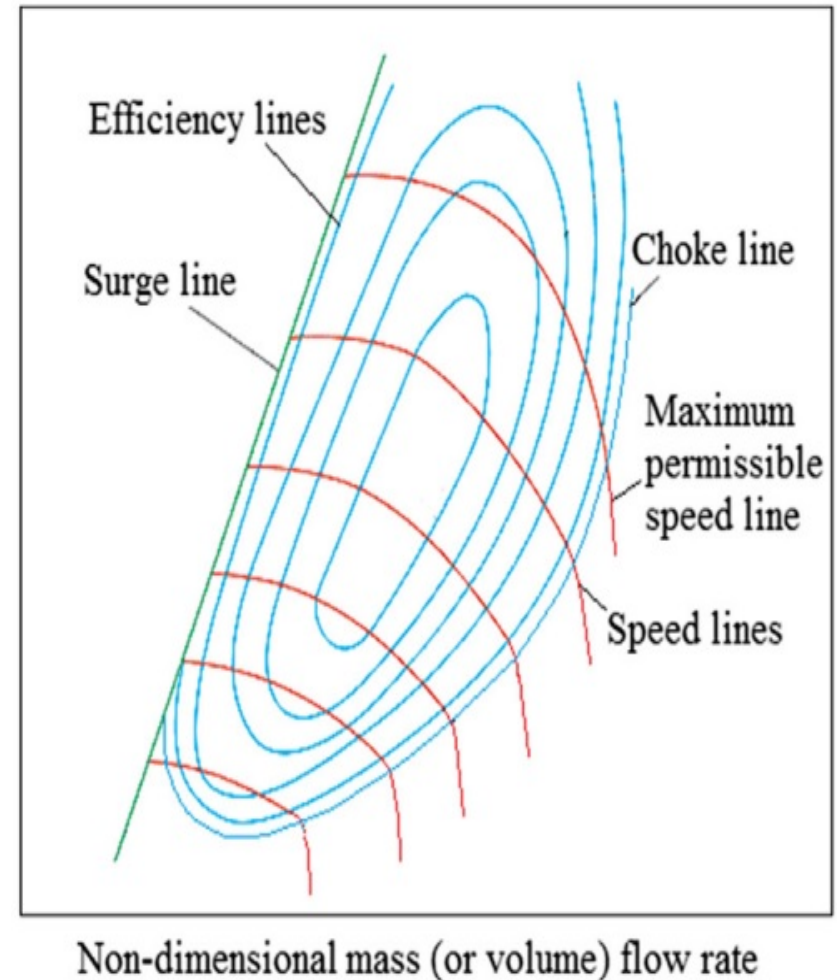
Thermodynamic Analysis

- **Implementation**
 - Console application written in **C#** uses **Coolprop** to evaluate properties
 - Optimization using **Matlab**
- **Minimum power: four stages**

| Fluid | rp1 | rp2 | rp3 | rp4 | W_{TOTAL} (kW) |
|---------------------------|---------------|---------------|---------------|---------------|---------------------|
| Pure CH ₄ | 3.5566 | 2.9894 | 2.5719 | 2.3940 | 49388 |
| Pure CO ₂ | 4.0318 | 2.9538 | 2.0274 | 2.6980 | 14684 |
| 70% CO₂ | 3.8284 | 3.0479 | 2.5264 | 2.2130 | 20340 |

1 D Analysis - Mean Line Method

- The Mean Line Method continues to be the best method for a first approach on centrifugal compressors design.
- A Mean Line code was implemented on MATLAB[®] software.
- The code is able to predict the centrifugal compressor performance faster than a CFD code with good accuracy.



1 D Analysis - Mean Line Method

The code was validated with experimental data for Air and Supercritical Carbon Dioxide (S-CO₂)

Air

| | Experimental Data | Mean Line Code | Relative Error % |
|----------------------|-------------------|----------------|------------------|
| Rotor Efficiency [-] | 0,880 | 0,880 | 0,00 |
| Pressure Ratio [-] | 2,176 | 2,081 | 4,37 |

Supercritical Carbon Dioxide

| | Experimental Data | Mean Line Code | Relative Error % |
|------------------------|-------------------|----------------|------------------|
| Outlet Temperature [K] | 378,9 | 376,93 | 0,52 |
| Outlet Pressure [kPa] | 24000 | 23540 | 1,92 |
| Pressure Ratio [-] | 2,5 | 2,48 | 0,80 |

Thermodynamic Properties of S-CO2

Thermophysical Properties of Fluid Systems

Accurate thermophysical properties are available for several fluids. These data include the following:

- Density
- Specific volume
- C_p
- C_v
- Enthalpy
- Entropy
- Internal energy
- Speed of Sound
- Viscosity
- Thermal conductivity
- Joule-Thomson coefficient
- Surface tension (saturation curve only)

Please follow the steps below to select the data required.

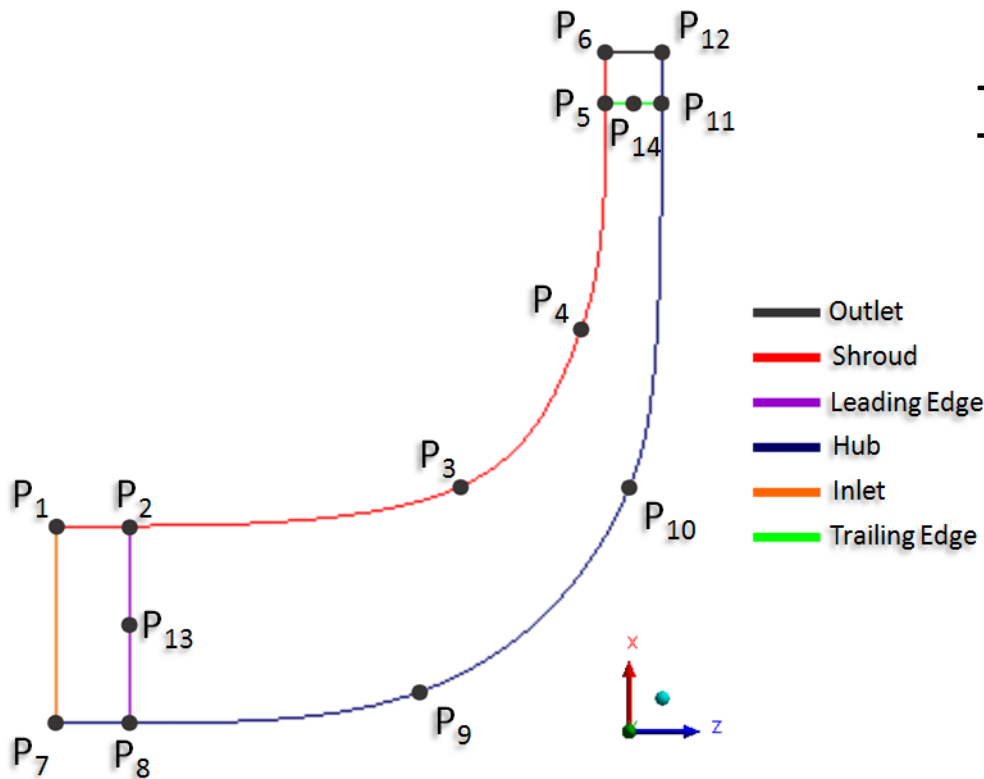
- Please select the species of interest:
- Please choose the units you wish to use:
Temperature: Kelvin Celsius Fahrenheit Rankine
Pressure: MPa bar atm. torr psia

```
File Edit View Search Tools Documents Help
DESCRIPTION
S-CO2 from NIST
NAME
SCO2
INDEX
SCO2
DATABASE
NIST REAL GAS PROPERTY DATABASE
MODEL
3
UNITS
1
PMIN_SUPERHEAT
7.600000E+006
PMAX_SUPERHEAT
3.000000E+007
TMIN_SUPERHEAT
3.000000E+002
TMAX_SUPERHEAT
1.100000E+003
SUPERCOOLING
0.000000E+000
P_CRITICAL
7.380000E+006
P_TRIPLE
5.185000E+005
T_CRITICAL
3.041800E+002
T_TRIPLE
2.165800E+002
GAS_CONSTANT
```

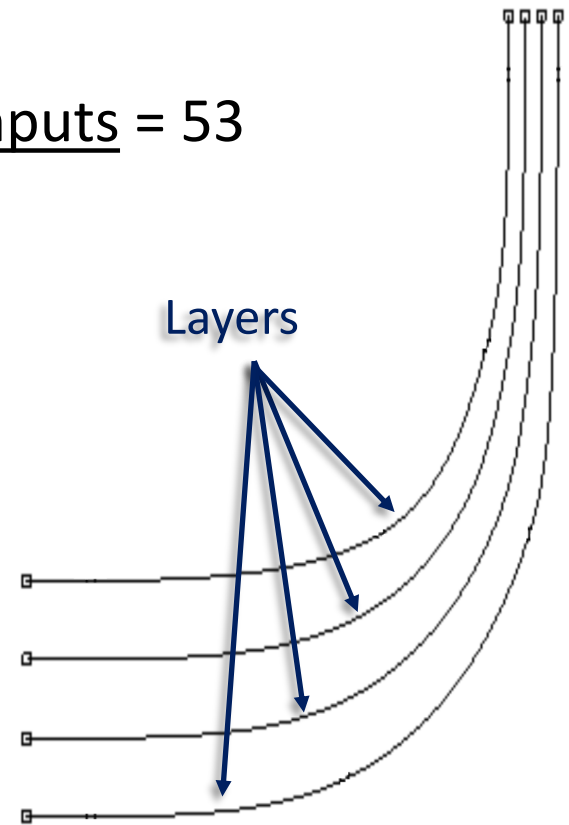
- Properties can be downloaded from NIST Website
- Converted through Matlab application to a RGP (Real Gas Properties) text file that can be used in ANSYS CFX

Blade Parametric Modeling for FVM

- **Geometry Input Variables:**

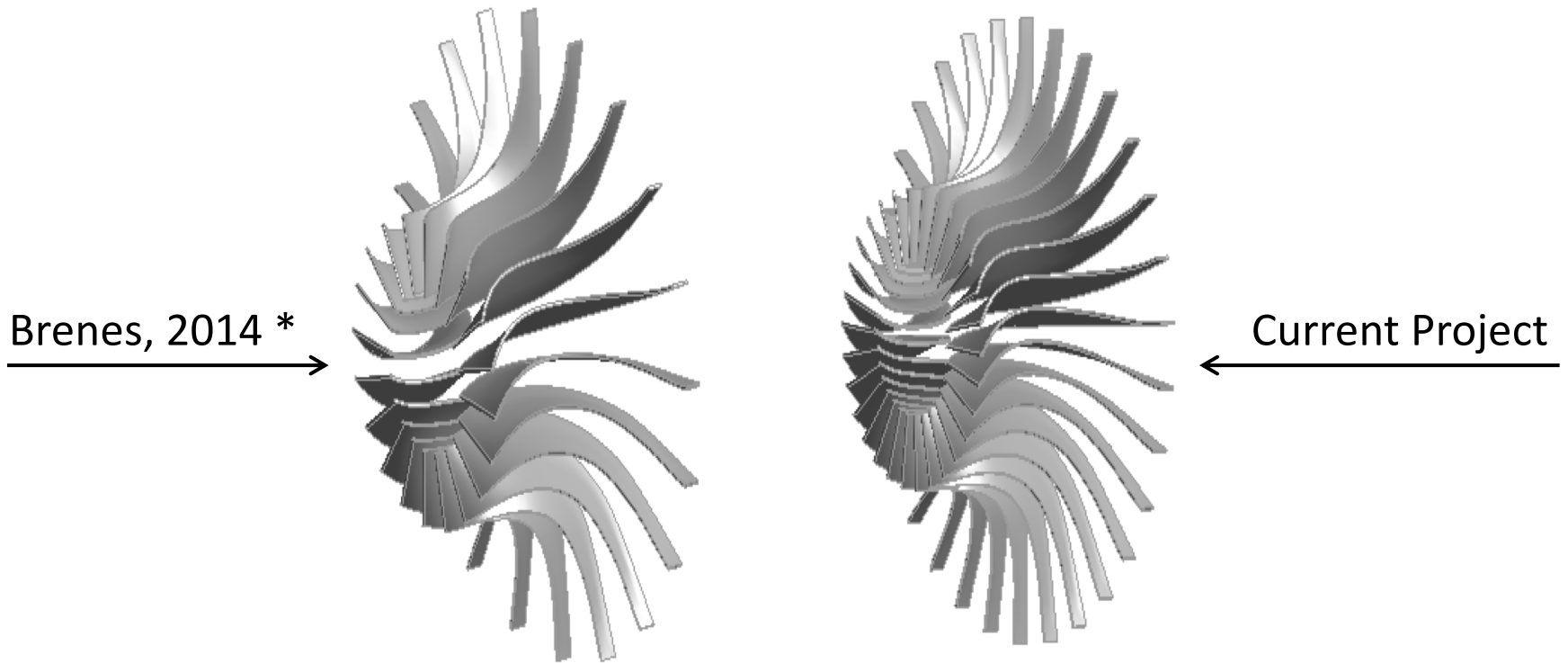


Total Inputs = 53



Centrifugal Compressor Modeling for FVM

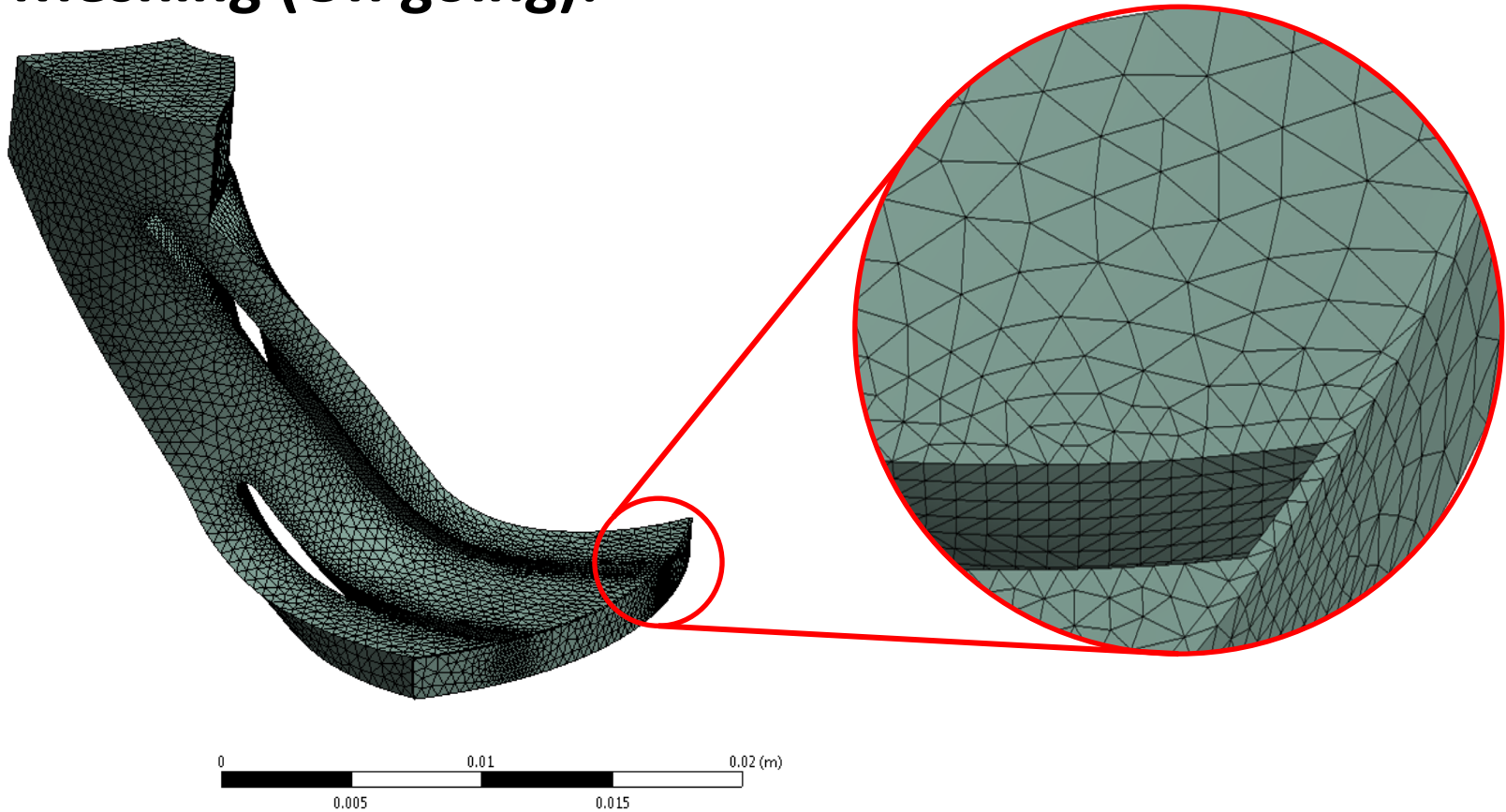
- **Geometry Input Variables:**



* Brenes, B.M., 2014. Design of supercritical carbon dioxide centrifugal compressors. University of Seville, Spain.

Centrifugal Compressor Modeling for FVM

- **Meshing (On going):**



FVM Simulation and Parametric Optimization

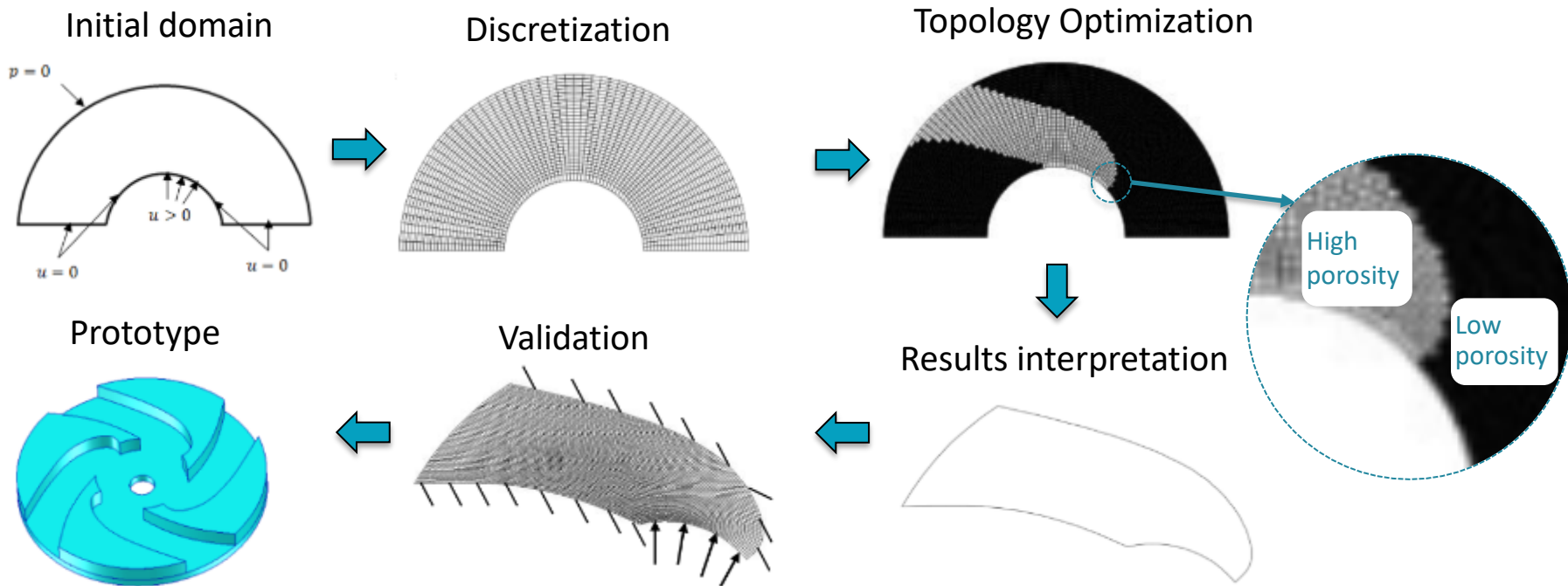
Next Steps:

- Coupling of 1D Software and ModeFrontier for 1D Optimization
- Implementation of Blade Parametric Modeling in the Vista CCD Software
- FVM software validation (turbulence model, meshing, S-CO₂ properties) using experimental data from the Sandia S-CO₂ Compressor

Topology Optimization

Determine material distribution in a design domain such that an objective function is extremized and constraints are fulfilled

Ex: rotating channel (aiming rotor design)



Topology Optimization

- Work is being developed in OpenFOAM
- Currently using Continuous Adjoint Method (sensitivities calculation)
- Optimization problem definition:

Minimize Energy dissipation /Pressure drop /Other functions

Subject to $\left\{ \begin{array}{l} \text{Navier Stokes + porosity field (design variables for TopOpt)} \\ \text{Volume constraint} \\ \text{Design variable constraint } (0 \leq \rho_{des} \leq 1) \end{array} \right.$

Porosity field represented by $\alpha \mathbf{u}$ in Navier Stokes equations

$\alpha = f(\rho_{des}) \rightarrow$ Porosity field controlled by ρ_{des}

Topology Optimization

- Example: design of a rotating channel minimizing energy dissipation (incompressible + without turbulence models)

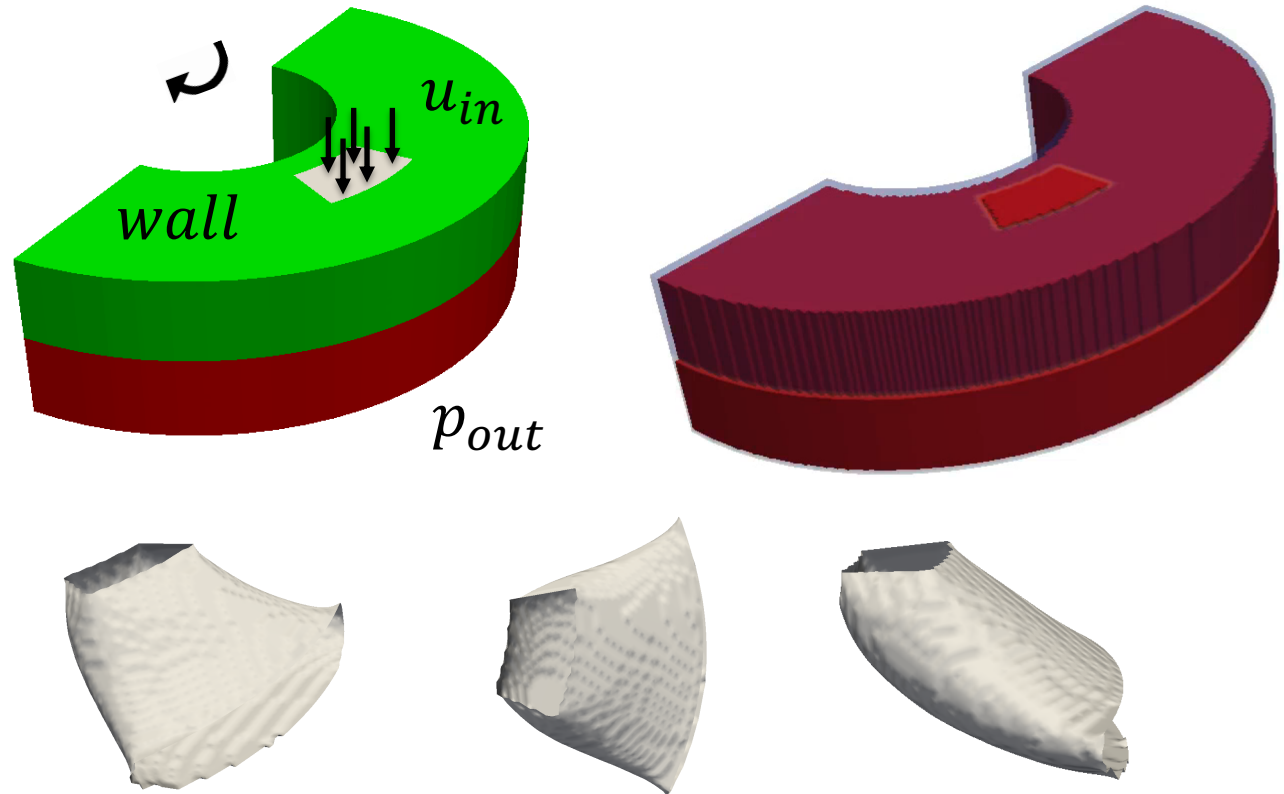
$$u_{in} = 1 \text{ m/s}$$

$$p_{out} = 0$$

$$\nu = 1 \text{ m}^2/\text{s}$$

$$\frac{\int \rho d\Omega}{\int d\Omega} = 20\%$$

$$\omega = 1000 \text{ rpm}$$



Topology Optimization

Next steps

- Cases with turbulence models are being studied, but improvements are necessary
- Assessment of Discrete Adjoint Method (sensitivities calculation)
- Optimize compressible flow cases



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