The EMPIR initiative is co-funded by the European Union's Horizon 2020 research and innovation programme and the EMPIR Participating States

MetHyInfra

EMPIR CALL 2020

Metrology infrastructure for high-pressure gas and liquified hydrogen flows

CFD Workshop

Part 2: CFD for Critical Flow Venturi Nozzles (CFVNs)

"Challenges, approaches and results"

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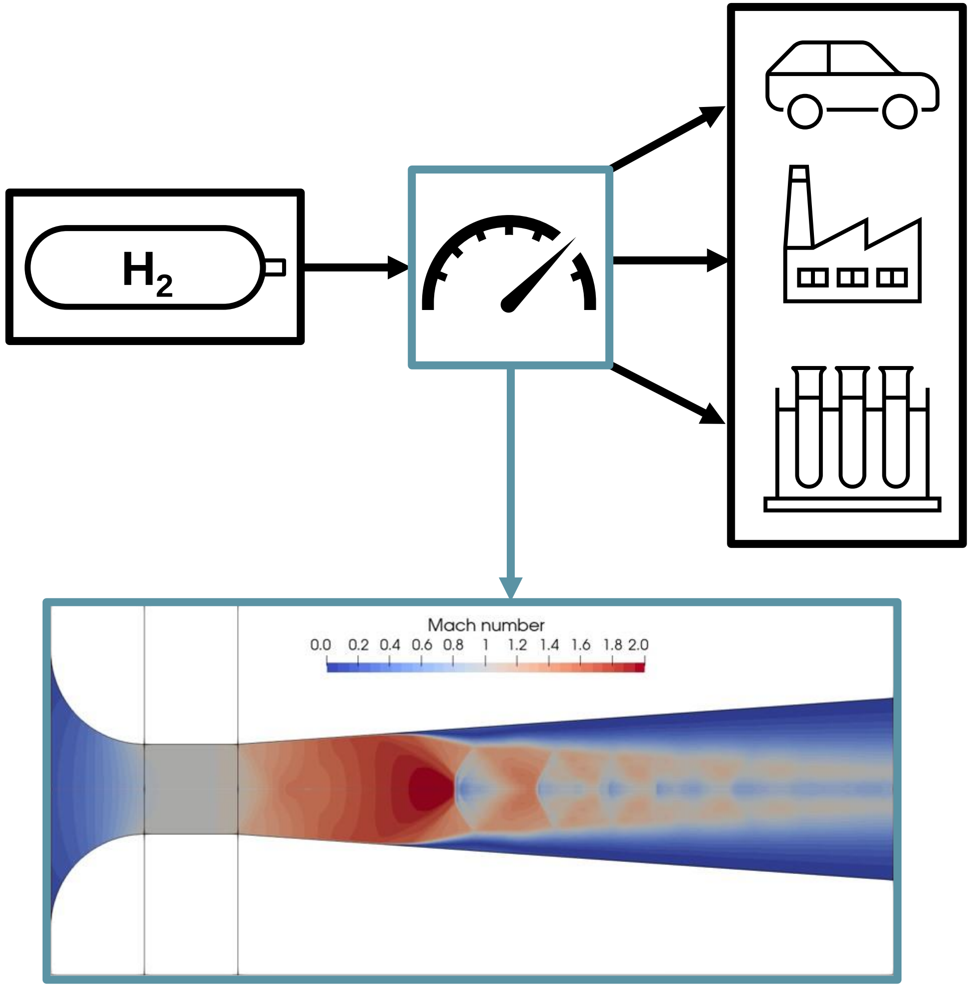
Working Groups 8.41 “Modelling and Simulation” and 1.45 “Hydrogen Quantity Metering”
Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany

Motivation

Hydrogen at high pressures

- promising energy carrier for use in climate-neutral applications in industry and transport
- needs to be stored at high pressures (up to 1000 bar) due to its low volumetric energy density

➢ to monitor hydrogen consumption, a verifiable flow measurement is required



Critical flow Venturi nozzles (CFVNs)

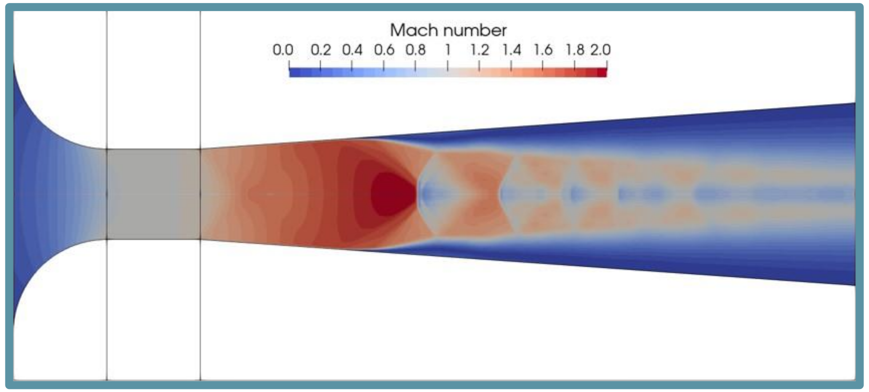
- state-of-the-art secondary standard gas flow meter
- gas accelerates to *Ma* = 1 (critical flow)
- international standards are limited to air and natural gases up to 200 bar

➢ **Flow simulation of hydrogen at high pressures**

CFD for high-pressure hydrogen flows

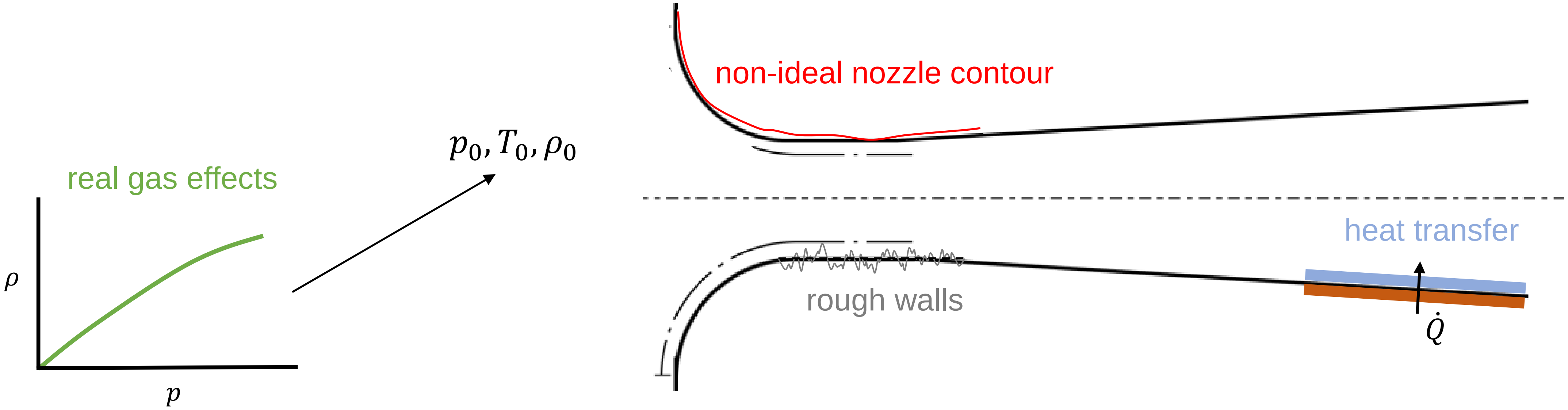
Aim:

Better understanding of the physics of
high-pressure hydrogen flows inside the nozzle



Need:

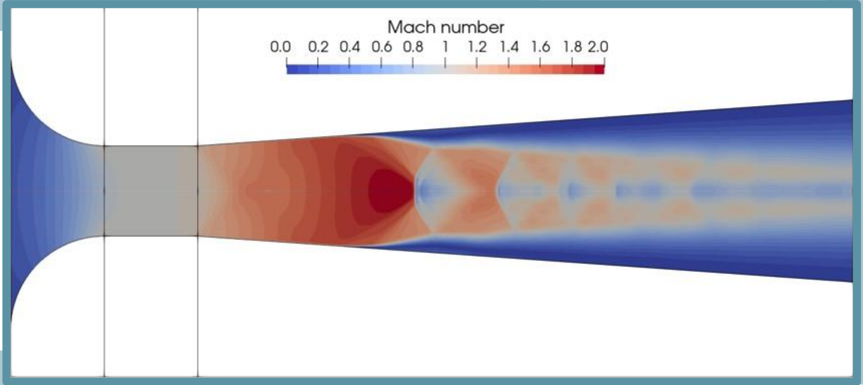
CFD model that takes the most relevant **real gas effects** into account,
modeling of **non-ideal, rough, and non-adiabatic walls**



Challenges

For a better understanding of the flow physics:

develop a CFD model that includes real gas effects, wall roughness, and heat transfer



Towards a “dry” calibration:

transform data
generated by dimensional
characterization
into parameters
of a CFD-applicable
computer model
of the physical process

For identifying the most significant parameters influencing the flow through critical nozzles:

perform efficient parameter studies
based on a validated CFD model

Approach

Start with simple model and extend it step by step:

- Choice of appropriate solver
- Choice of appropriate turbulence model
- Inclusion of real gas effects
- Consideration of non-ideal shapes and rough walls
- Consideration of non-adiabatic walls

Start with studying the influence of different parameters / effects systematically before considering specific nozzles / setups

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Approach

Real gas model

Surrogate model

1. Study the influence of different parameters systematically

Choice of turbulence model

Parametrized shape (toroidal → cylindrical)

Rough walls

Heated walls

Validation with existing data
(e.g., from the literature)
or with experiments designed for this purpose

3. Substitute CFD model by cheaper surrogate model

→ allows to study systematic influence of various parameter combinations

→ basis for the “dry” calibration of nozzles

2. Modeling specific nozzles / settings
(e.g., from the MetHyInfra project)

Dimensional charac-terization of nozzles
→ real shape
→ roughness level

Operating conditions

Boundary conditions on wall

Validation with corresponding experiments

Realization in MetHyInfra project

CFD work summarized in **one work package**

- Title: **“Development of a CFD model for high pressure hydrogen flows”**
- Partners involved: **PTB, ESI**
- Work divided into **4 tasks**

Task 1:
Literature review and strategy for CFD modeling

Task 2:
CFD model for critical nozzle flows

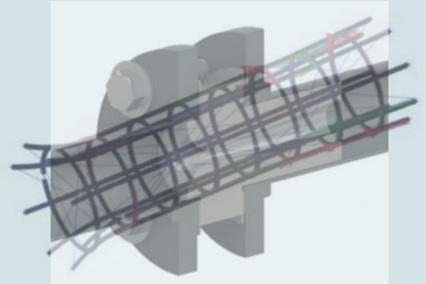
Task 3:
CFD model for high pressure hydrogen flows

Task 4:
Influence of rough and non-adiabatic walls

Interaction with other parts of the project

METAS:

Dimensional characterization of nozzles



real shape

+ known roughness

NEL, Cesame, JV, METAS, MH, UL:

Experiment

$c_{D,\ \mathrm{exp}}$

Comparison

Validation

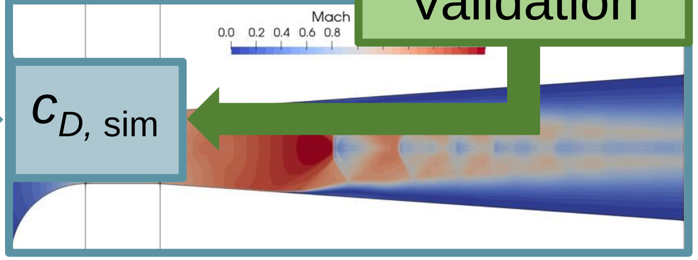
ESI, PTB:

Parametrized mesh

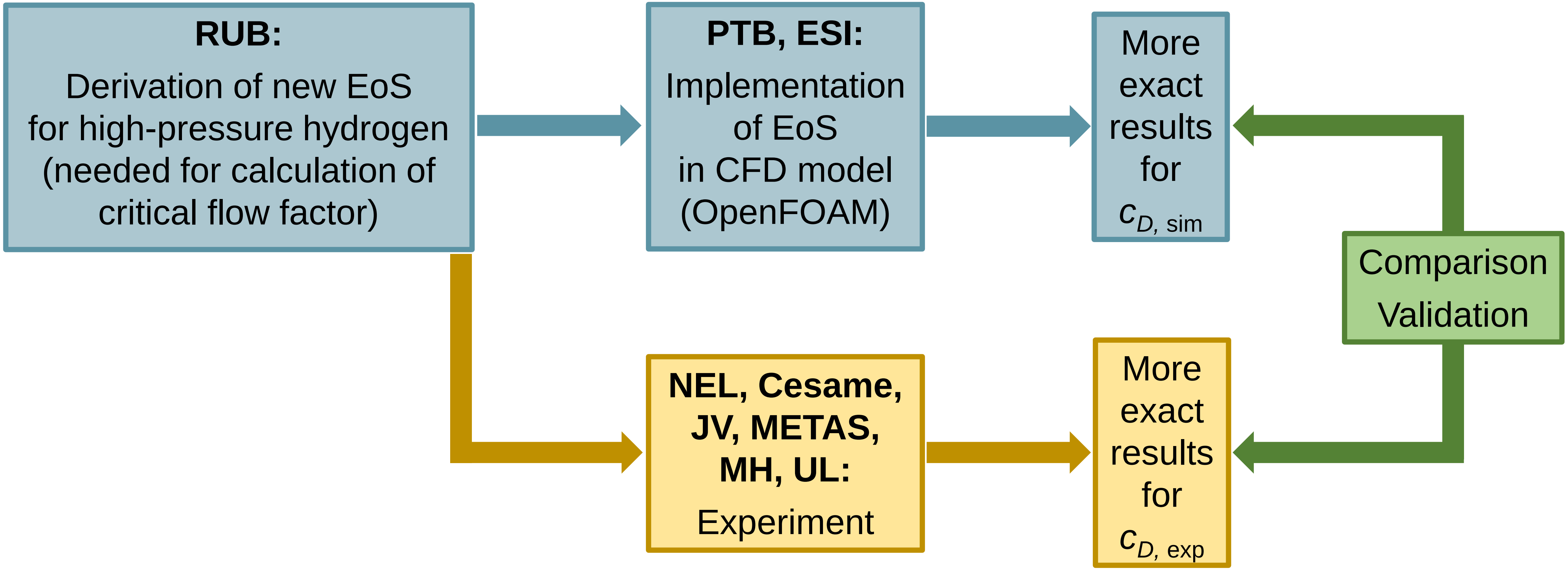
PTB, ESI:

CFD model

$c_{D,\ \mathrm{sim}}$



Interaction with other parts of the project



Realization in MetHyInfra project

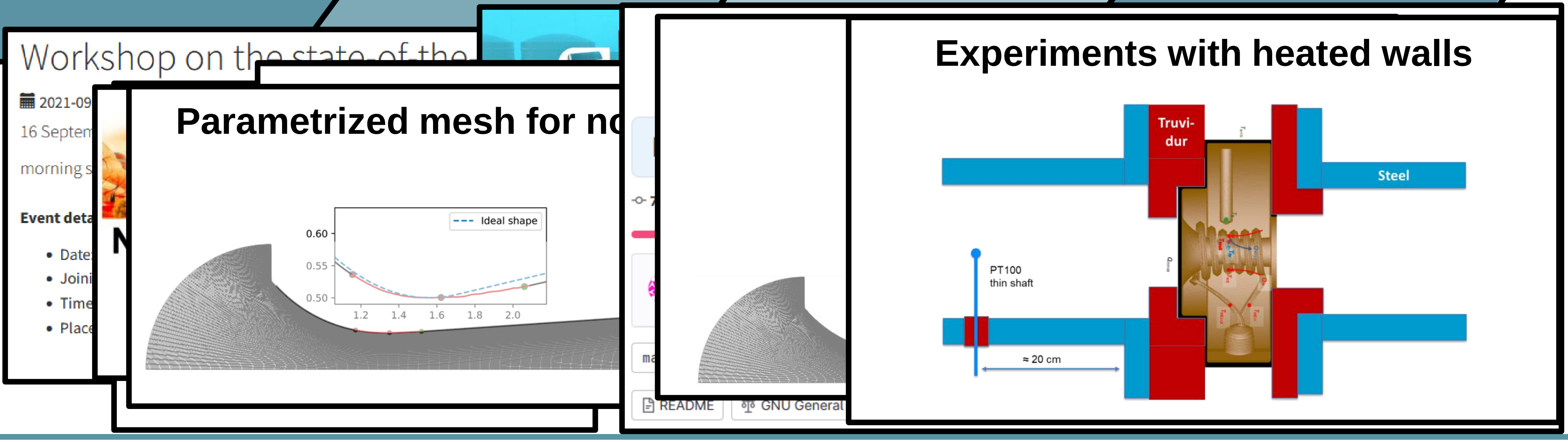
Development of a CFD model for high pressure hydrogen flows

Task 1:
Literature review and strategy for CFD modeling

Task 2:
CFD model for critical nozzle flows

Task 3:
CFD model for high-pressure hydrogen flows

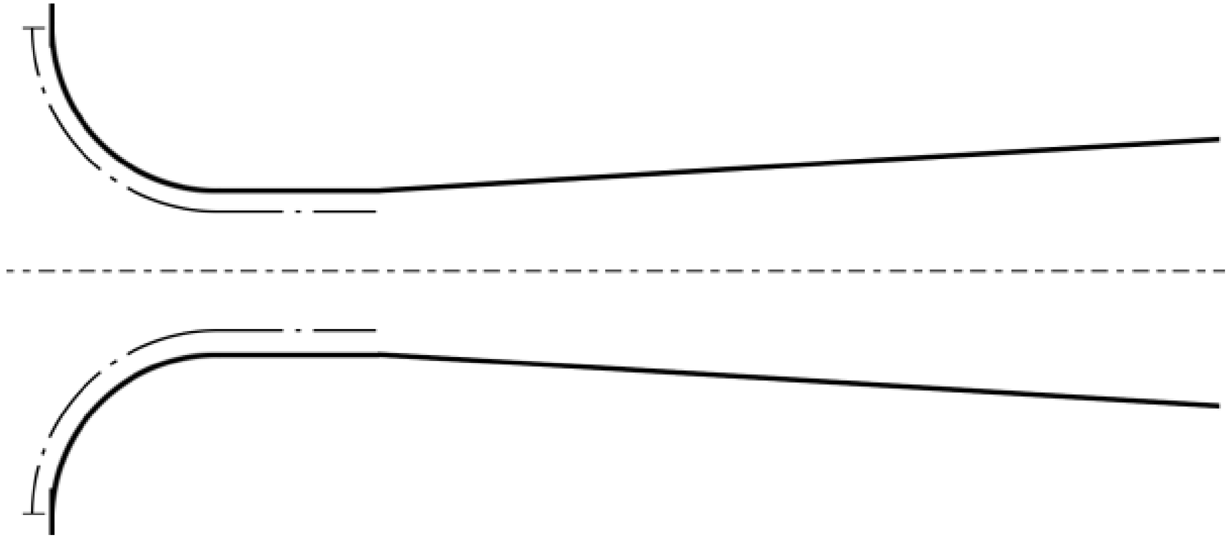
Task 4:
Influence of rough and non-adiabatic walls



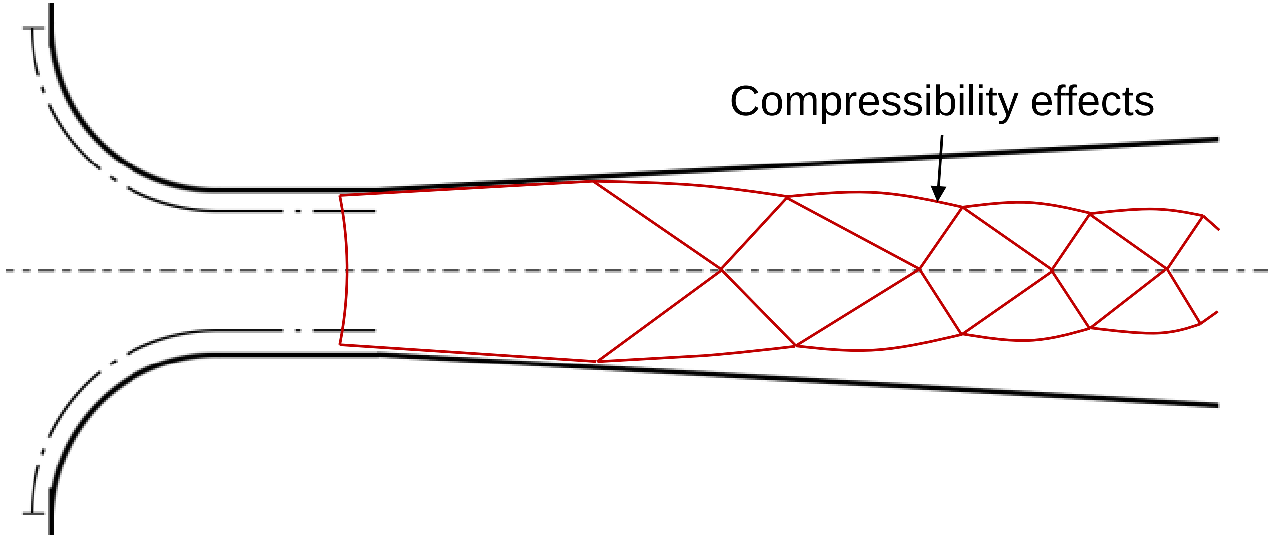
Results

Come back to CFVN (critical flow Venturi nozzle)

and consider different effects

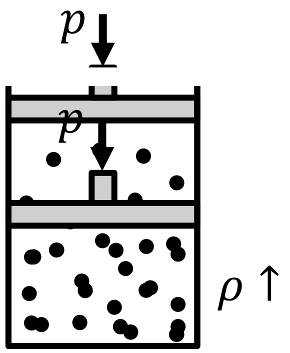


Compressibility effects



Compressibility effects

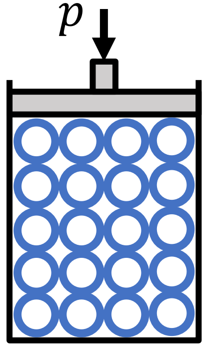
Compressible fluid



$$a_{compr.} = \sqrt{\kappa R_M T} \quad \text{(Ideal gas)}$$

- Fluid properties change after arrival of sound wave

Incompressible fluid

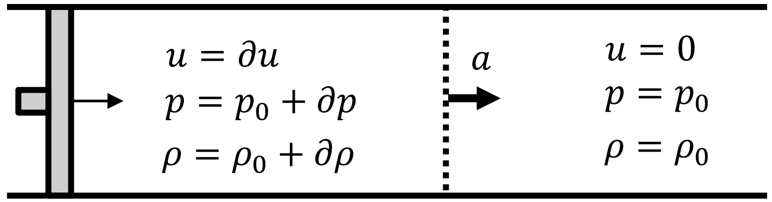


$$a_{incompr.} \to \infty$$

- Fluid properties change instantaneously

Speed of sound

- Propagation velocity of small pressure disturbances in a medium



Piston moves at velocity ∂u

Wave moves away from piston at velocity a

- From conservation law of mass and momentum, the speed of sound can be derived as

$$a = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s}$$

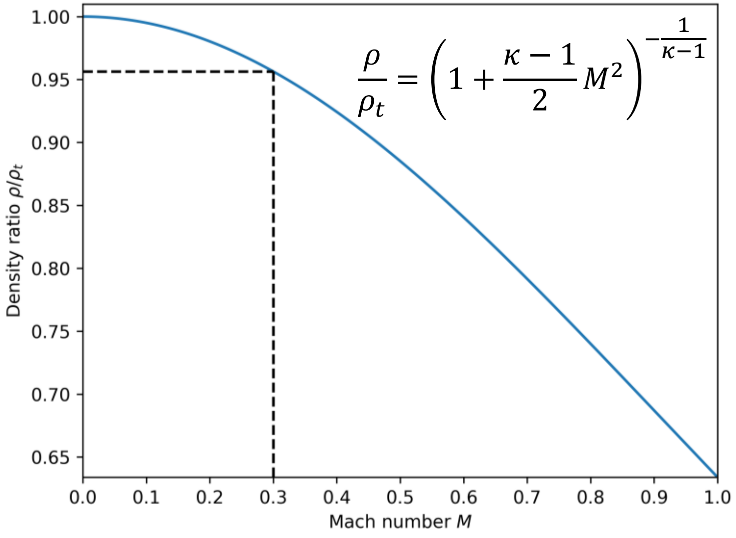
Compressibility effects

Mach number

- Ratio of flow velocity to local speed of sound

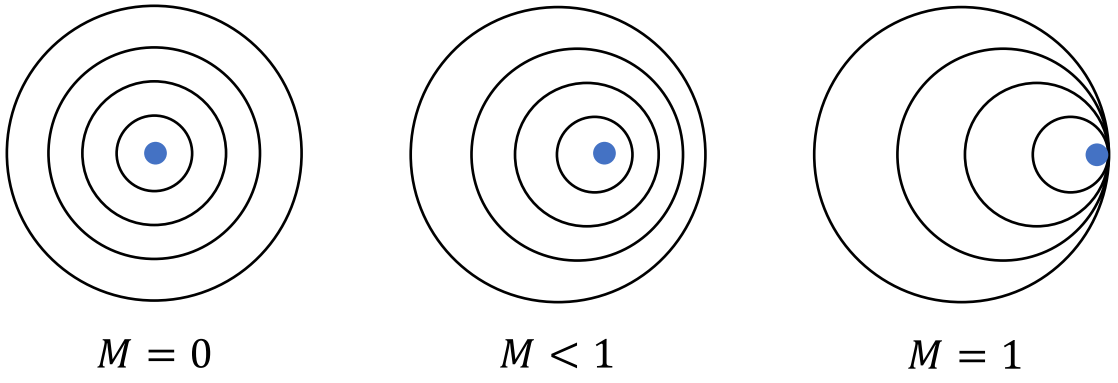
$$M = \frac{u}{a}$$

- Typically, flows are considered compressible when Mach number exceeds 0.3



- At *M = 0.3*, change in density is ca. 5% and can't be neglected

- What happens when flow reaches *M = 1*?

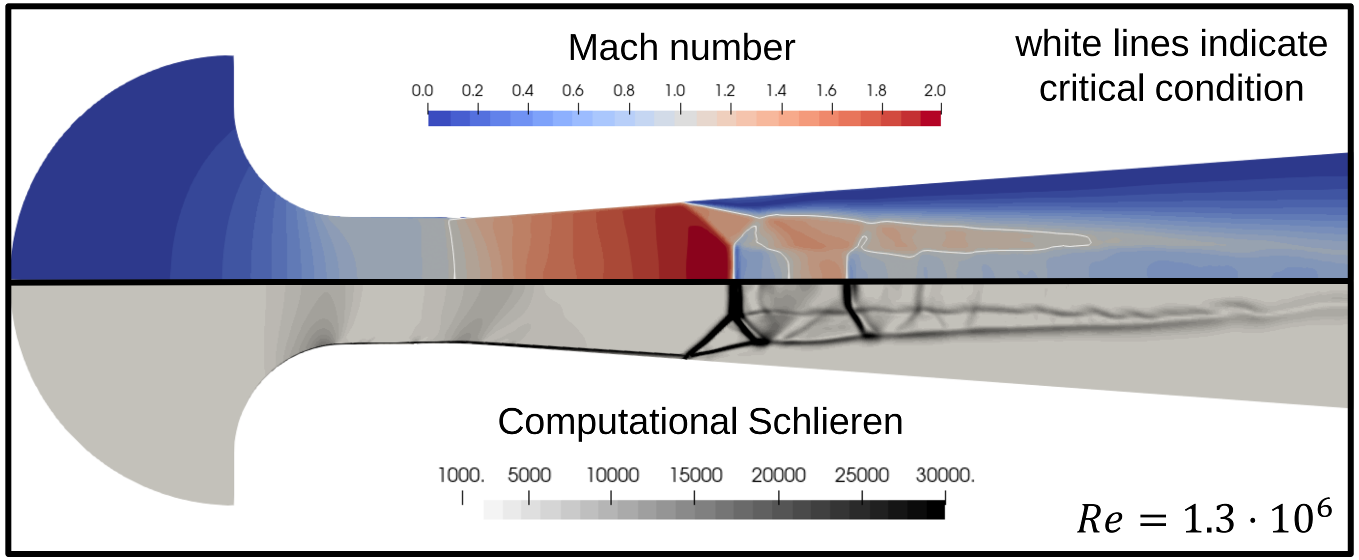


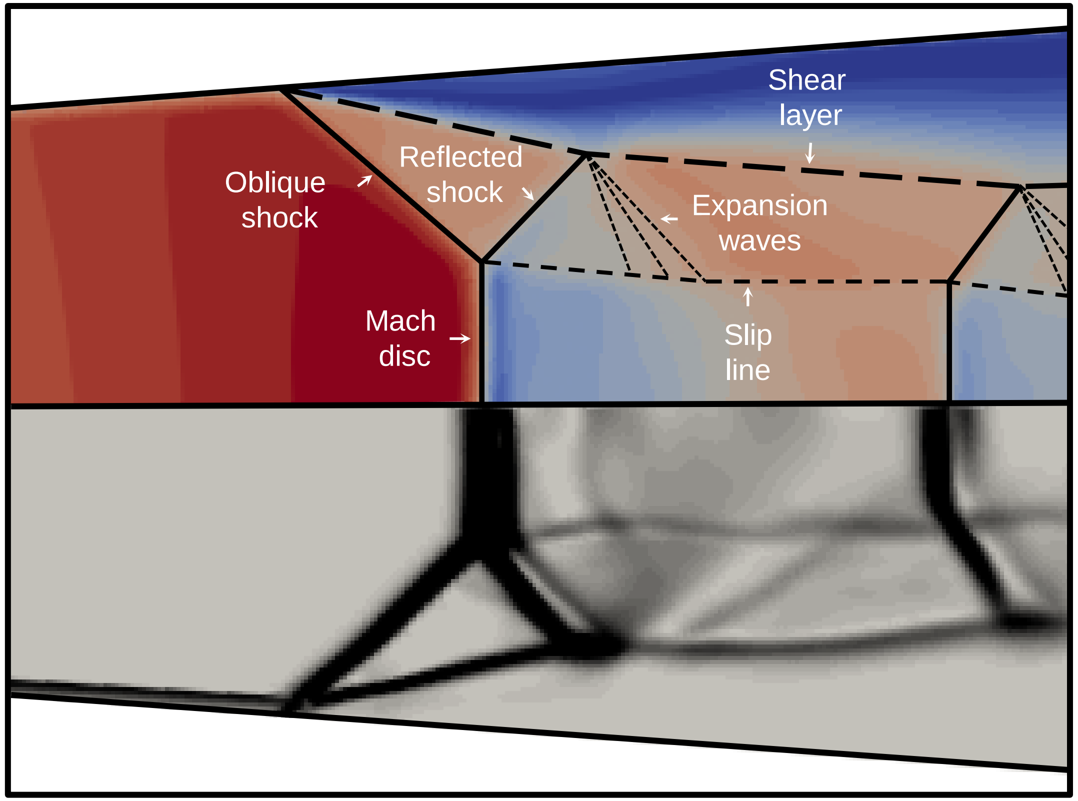
- Waves in front of object get compressed
- In flows, where *M ≥ 1*, small disturbances can't propagate upstream
- In the context of critical nozzles:
  - Flow rate only depends on upstream conditions

Compressibility effects

- A compressible flow solver is used for the critical nozzle flow
  - ➢ here: sonicFOAM

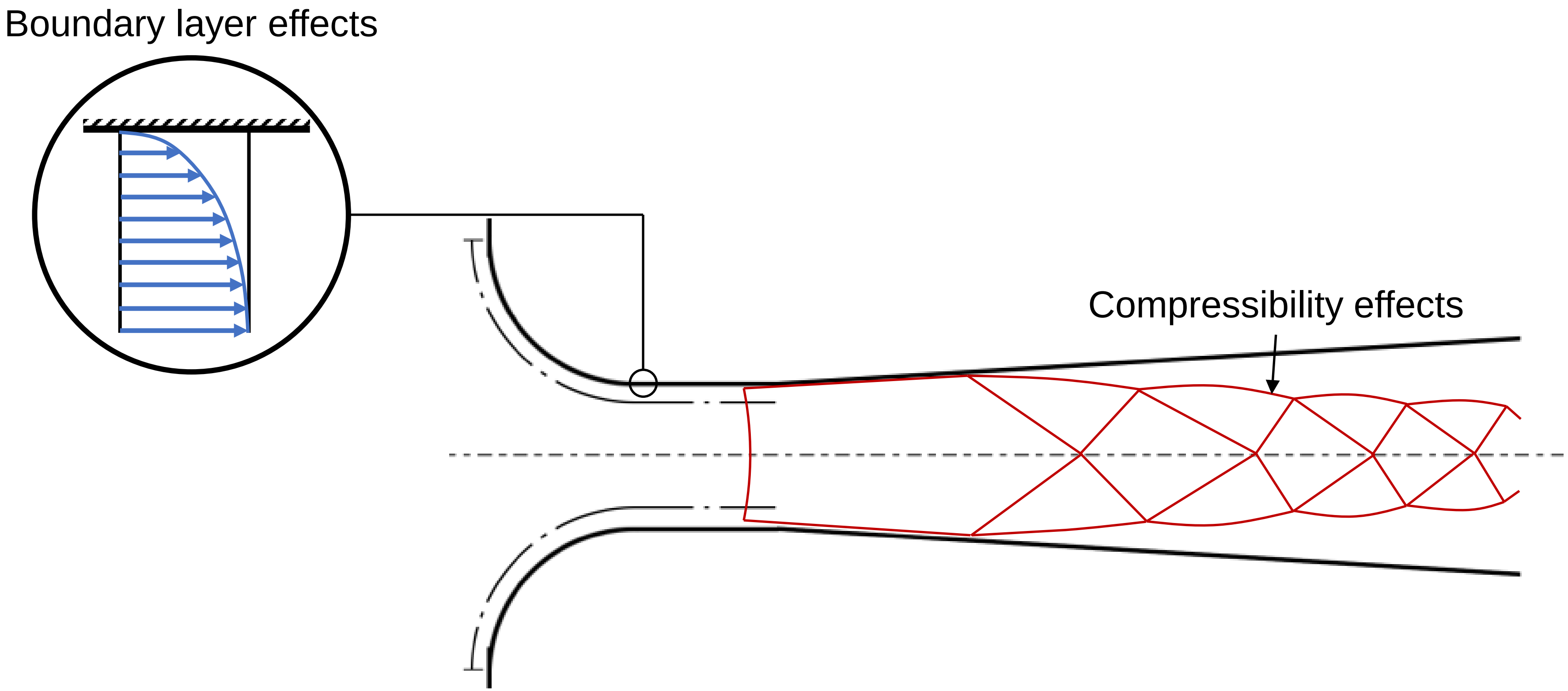
- Let's have a look at the flow field





➢ Critical flow (*Ma* = 1) is reached in nozzle throat (see white line)

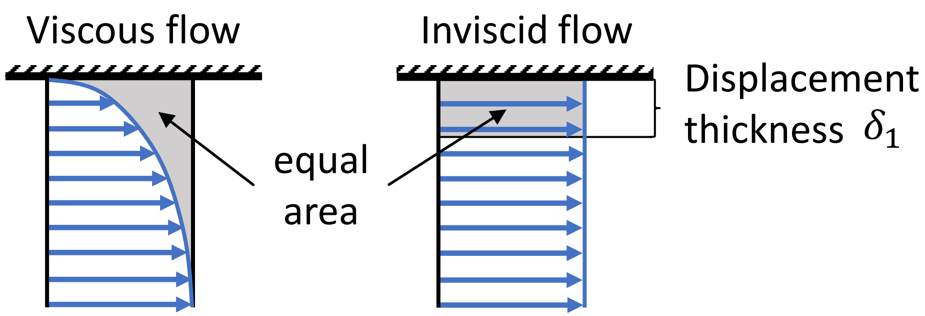
Boundary layer effects



Boundary layer effects

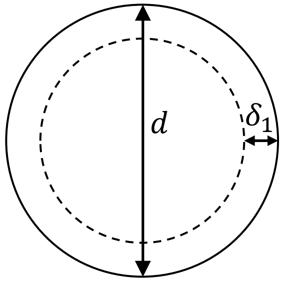
Boundary layer (BL)

- ➢ thin region close to wall, where viscous effects on velocity profile are significant



Displacement thickness

- ➢ reduces effective cross-sectional area



$$C_D \sim \left(1 - \frac{2\delta_1}{d}\right)^2$$

Reynolds number

- ➢ Ratio of inertial to viscous forces

$$Re = \frac{\rho u d}{\mu}$$

Laminar BL

- Smooth, rectified flow
- Occurs at lower *Re* values
- ➢ Viscous forces dominate

Turbulent BL

- Chaotic, swirling flow
- Occurs at higher *Re* values
- ➢ Inertial forces dominate

- In CFD, RANS turbulence models with wall functions are used
- ➢ How is turbulence actually modeled?
- ➢ And what are wall functions for?

Turbulence modeling (1)

- Navier Stokes equations (incompressible, easier to explain):

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_i u_j\right) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right]$$

- Reynolds-averaged Navier Stokes (RANS) equations:

$$\frac{\partial(\rho \bar{u}_i)}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho \bar{u}_i \bar{u}_j\right) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) - \rho\overline{u_i' u_j'}\right]$$

Reynolds decomposition

$$u(\boldsymbol{x},t) = \bar{u}(\boldsymbol{x}) + u'(\boldsymbol{x},t)$$
$$p(\boldsymbol{x},t) = \bar{p}(\boldsymbol{x}) + p'(\boldsymbol{x},t)$$

Mean component

Fluctuating component

- The Reynolds-averaging process results in an additional stress term:

$$-\rho\overline{u_i' u_j'}$$

- In order to solve the RANS equations, we need to express the Reynolds stress in terms of the mean flow quantities

➢ This is the turbulence closure problem

Turbulence modeling (2)

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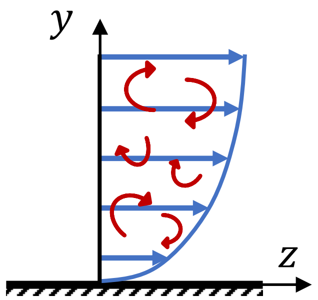
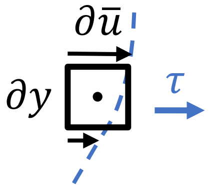
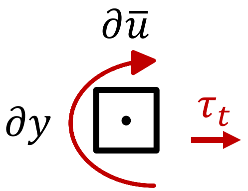
- Consider a simple turbulent shear flow in 2D (like close to the wall of the nozzle):





Mean flow



Eddy

➢ The fluid element is sheared by the mean flow and by the eddy

Shear stress from mean flow (viscous shear):

$$\tau = \mu \frac{\partial \bar{u}}{\partial y}$$

Shear stress from eddies / turbulence is given by Reynolds stress:

$$\tau_t = -\rho \overline{u'v'}$$

<u>Eddy viscosity model (or Boussinesq‘s hypothesis:)</u>

$$\boxed{-\rho \overline{u'v'} = \mu_t \frac{\partial \bar{u}}{\partial y}}$$

with eddy / turbulent viscosity μ_t

➢ μ_t needs to be modeled in turbulence model

General form

$$-\rho \overline{u_i' u_j'} = \mu_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} k \delta_{ij}$$

μ_t is considered isotropic

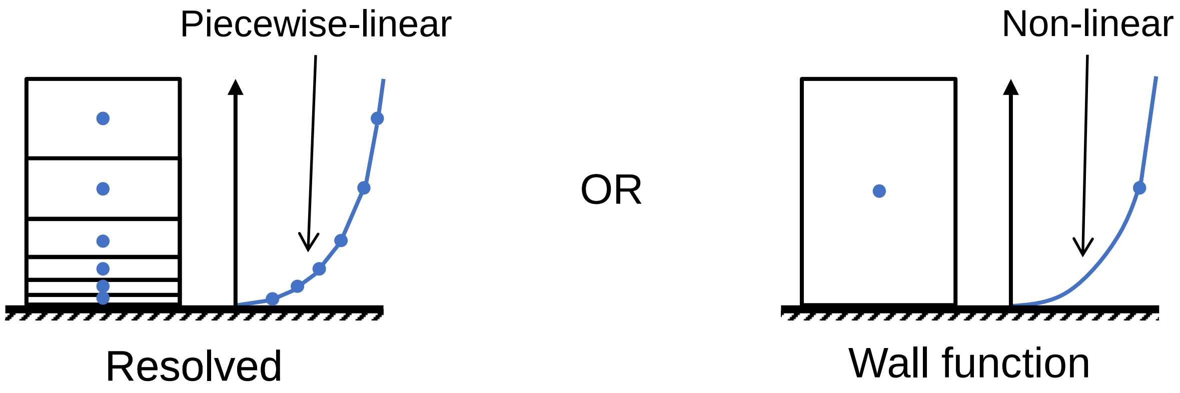
Turbulence modeling (3)

k-ω Shear Stress Transport (SST) model

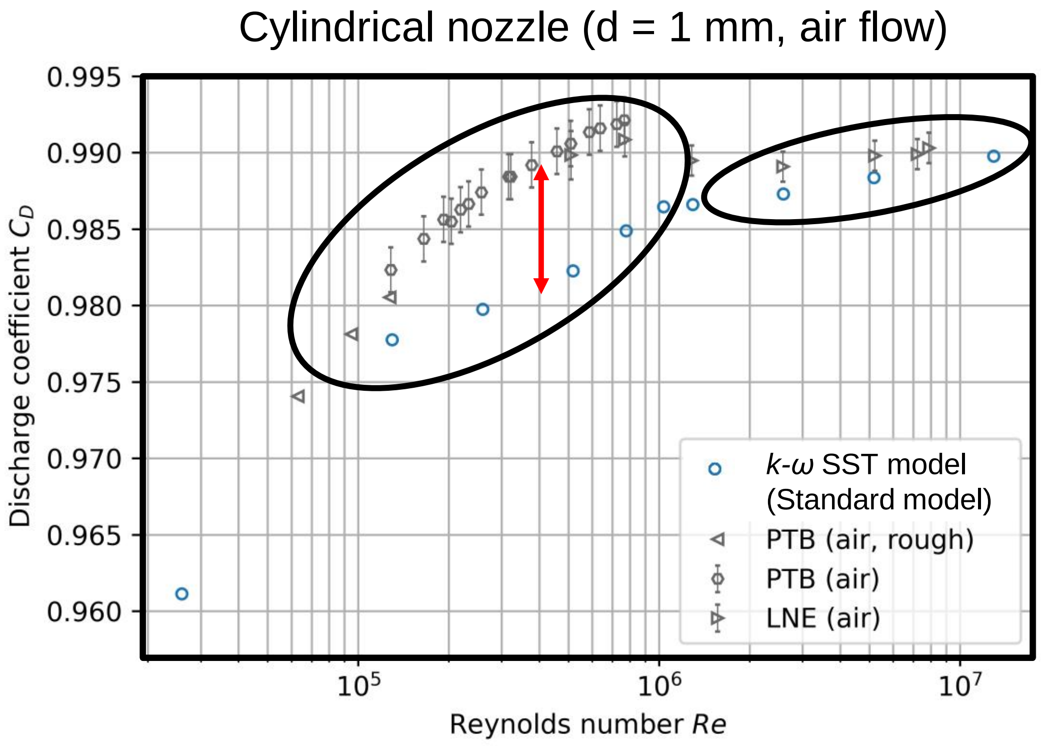
- In order to determine eddy viscosity, two additional transport equations are solved:
  - Turbulence kinetic energy *k*
  - Turbulence specific dissipation rate *ω*
- Combines strenghts of *k-ω* model (inner region of boundary layer) and *k-ε* model (free stream)

Automatic wall treatment

- Depending on y+ value (dimensionless wall distance):

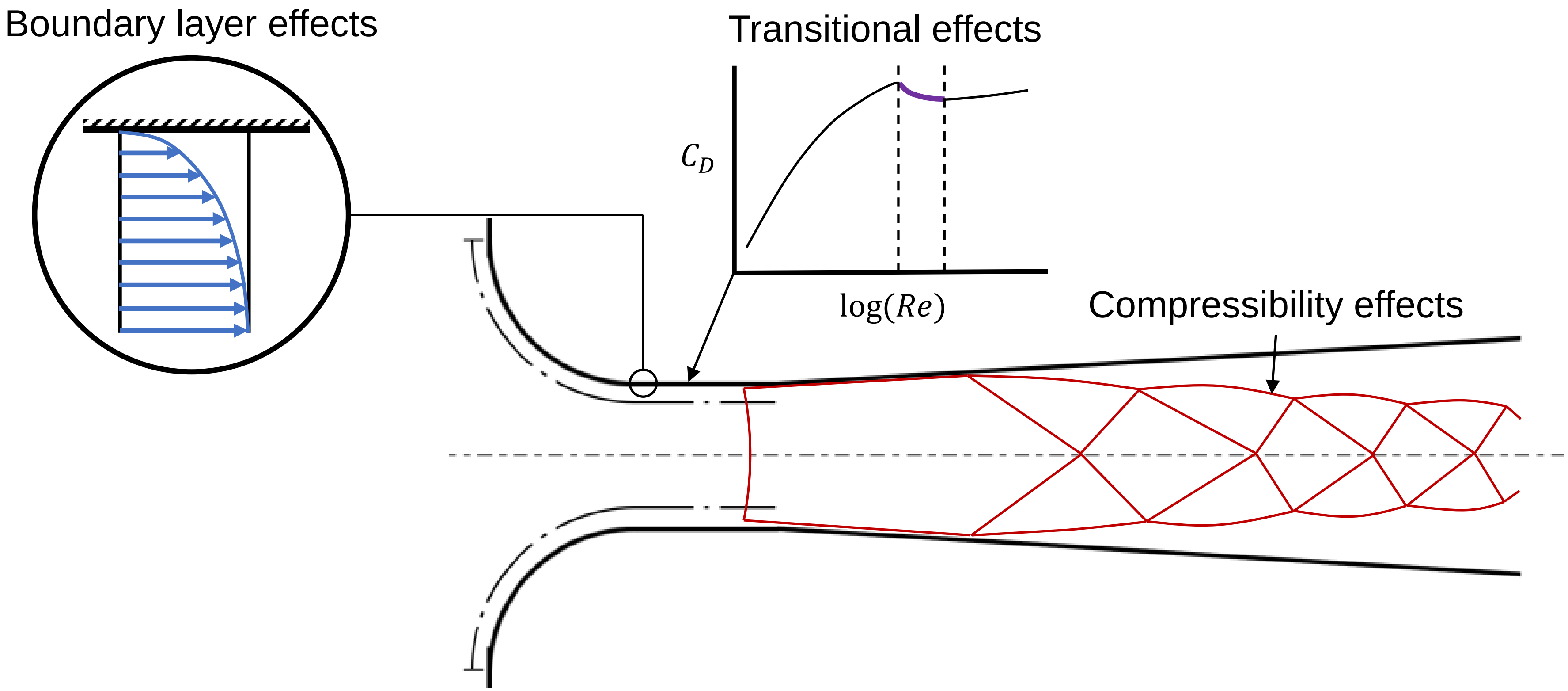


Results



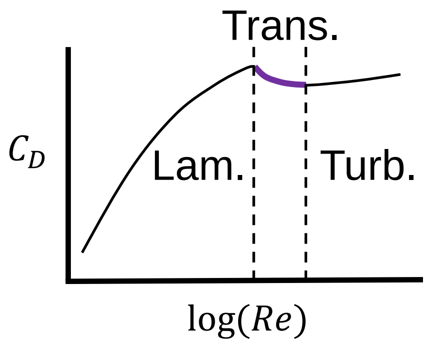
- Performs well for high Re numbers (turbulent region)
- Underperforms for low Re numbers (laminar region)
- ➢ Better predictive model required

Transitional effects



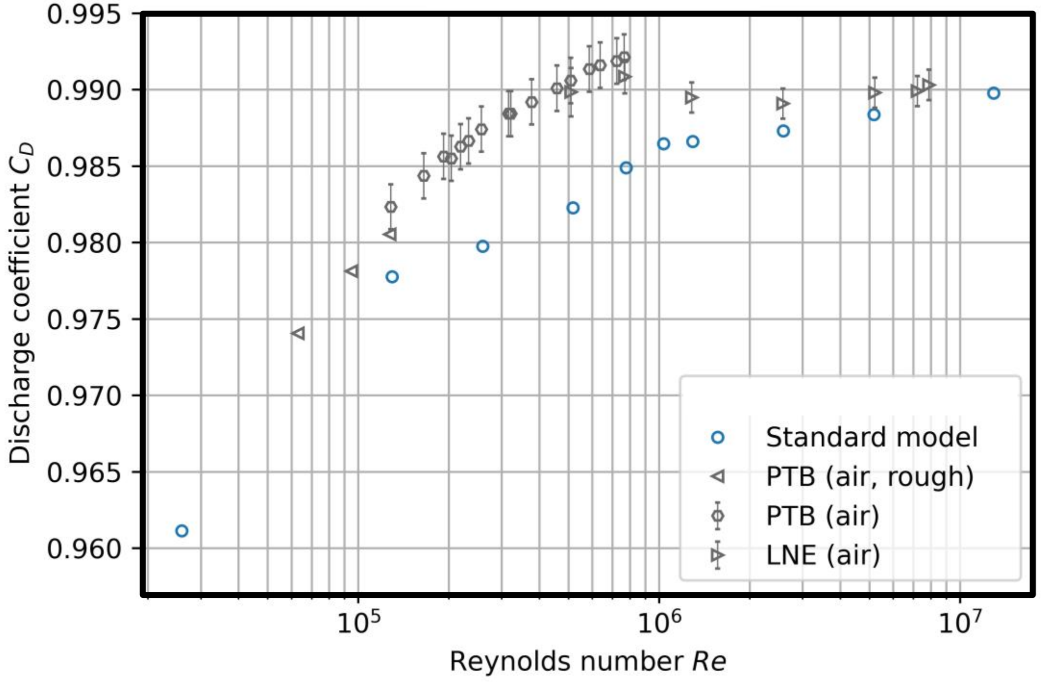
Transitional effects

- Transition describes the process of a laminar boundary layer becoming turbulent
- It occurs in a specific Reynolds number *Re* range (typically at *Re* = 10^6 for CFVNs)



- In CFD, transitional turbulence model uses trigger parameter γ to model transition process, where
  - $\gamma = 0$ for laminar flow
  - $\gamma = 1$ for turbulent flow
  - $0 < \gamma < 1$ for transitional flow

Cylindrical nozzle (d = 1 mm, air flow)



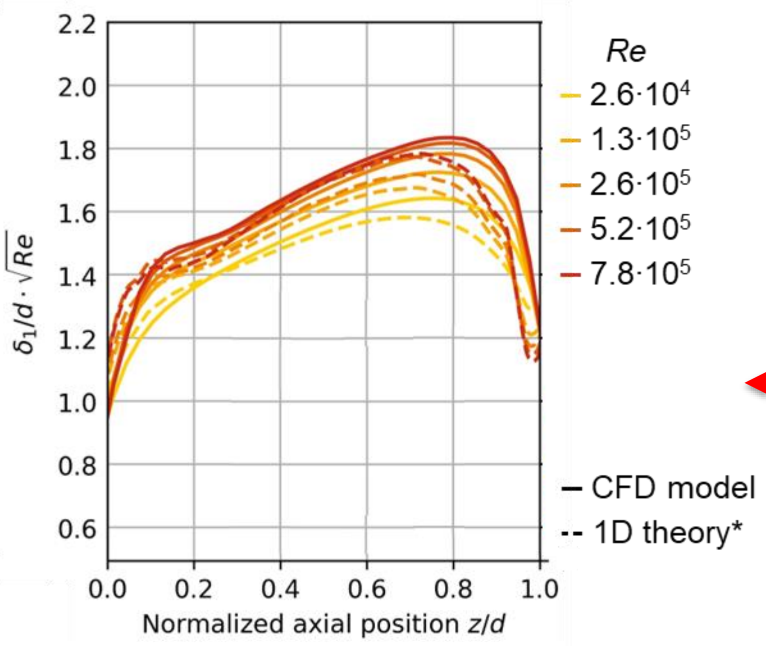
- ○ Standard model in good accordance with experimental data for higher *Re*
- ◇ Transitional model in good agreement in entire *Re* range

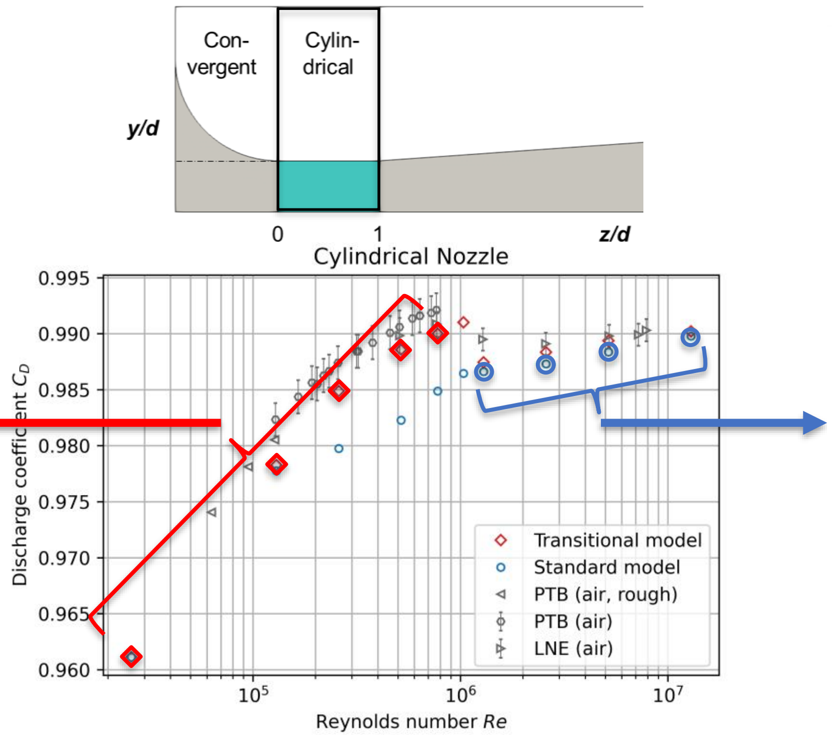
Displacement thickness

Definition

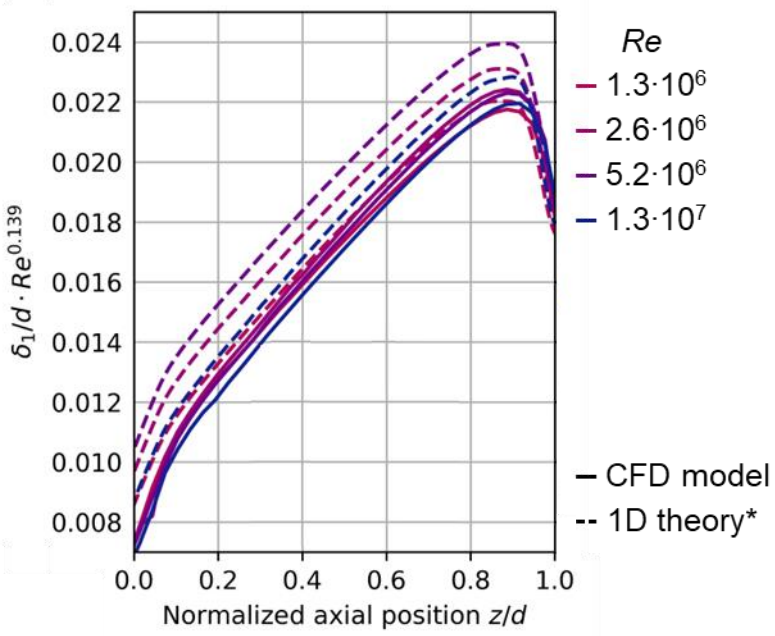
$$\delta_1 = \int_0^{\delta_{max}} \left(1 - \frac{\rho U}{(\rho U)_{max}}\right) dy$$

Laminar region





Turbulent region

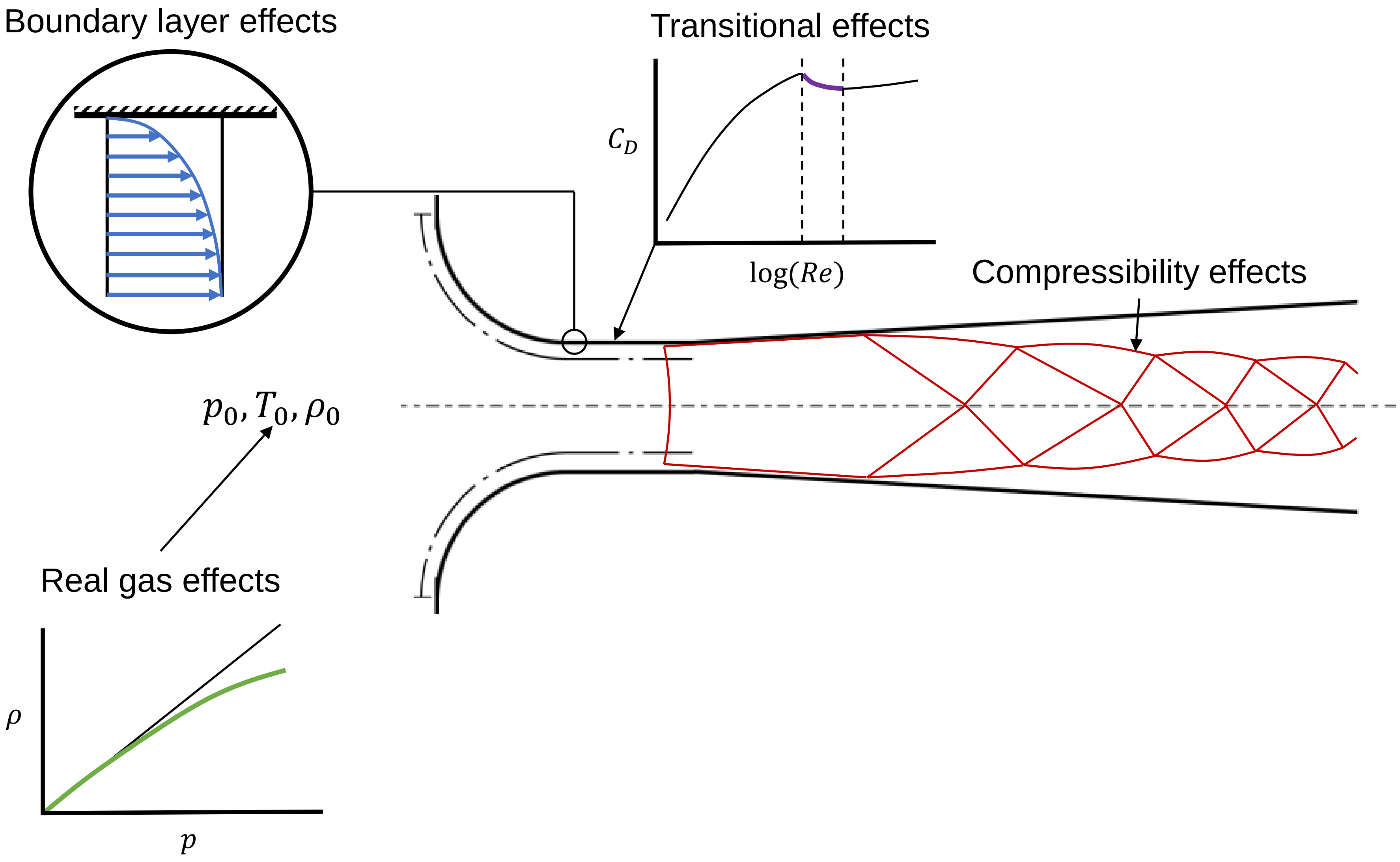


Self-similar for $\sqrt{Re}$

* Based on integral methods for solving the boundary layer equations (by B. Mickan)

Self-similar for $Re^{0.139}$

Real gas effects



Real gas effects

Motivation

What is the difference between a real and an ideal gas?	
Ideal gas Particles have no volume Collisions are elastic No interactions between particles	Real gas Particles have volume Collisions are non-elastic Intermolecular forces
Real gases behave like ideal gases: At high temperatures At low pressures	

- Nozzle flow for pressures up to 100 MPa needs to be considered
- ➢ Real gas effects are relevant and cannot be neglected
- ➢ Consideration of appropriate real gas model in CFD simulation

	Ideal gas model	Real gas model (e. g. Peng-Robinson)
Equation of State (EoS)	$p \cdot V_m = R \cdot T$	$\left(p + \underbrace{\frac{\alpha \cdot a}{V_m^2 + 2b \cdot V_m - b^2}}_{\text{allows for intermolecular forces}}\right) \cdot (V_m - \underbrace{b}_{\text{allows for effect of particle volume}}) = R \cdot T$ ➢ already available in OpenFOAM

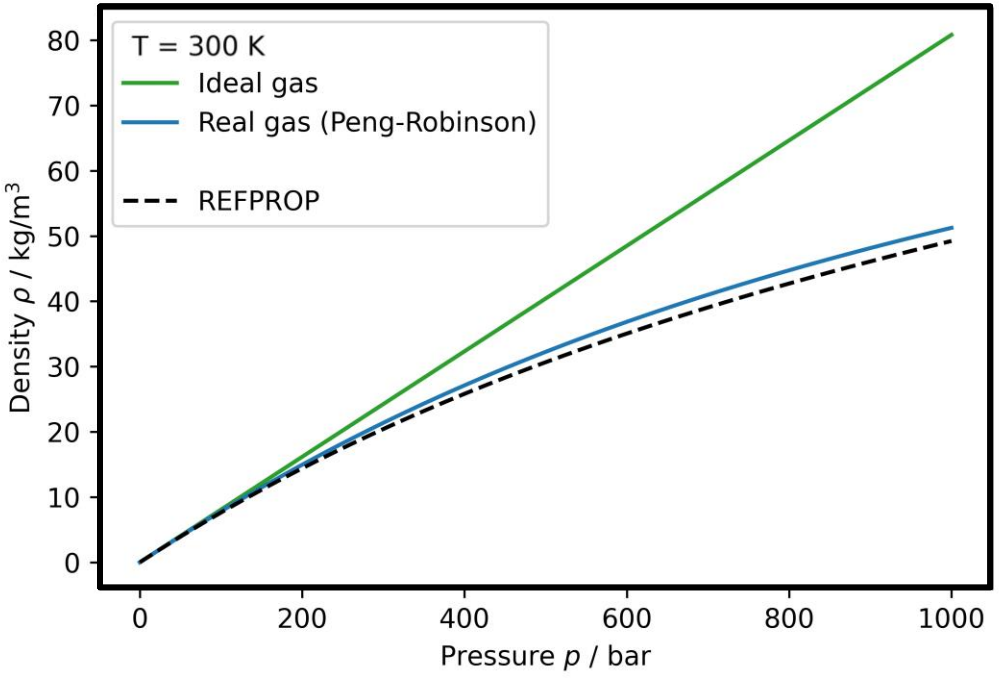
Real gas effects

Real gas model

- High deviation in density at high pressures between
  - Ideal gas (–) and
  - real gas (**---**)
- Real gas model of Peng & Robinson (–) is available in OpenFOAM
  - However, deviation is still up to 5 % from REFPROP

➢ A more precise real gas model for hydrogen is implemented based on REFPROP data

Hydrogen



Real gas effects

New model

Full temperature range

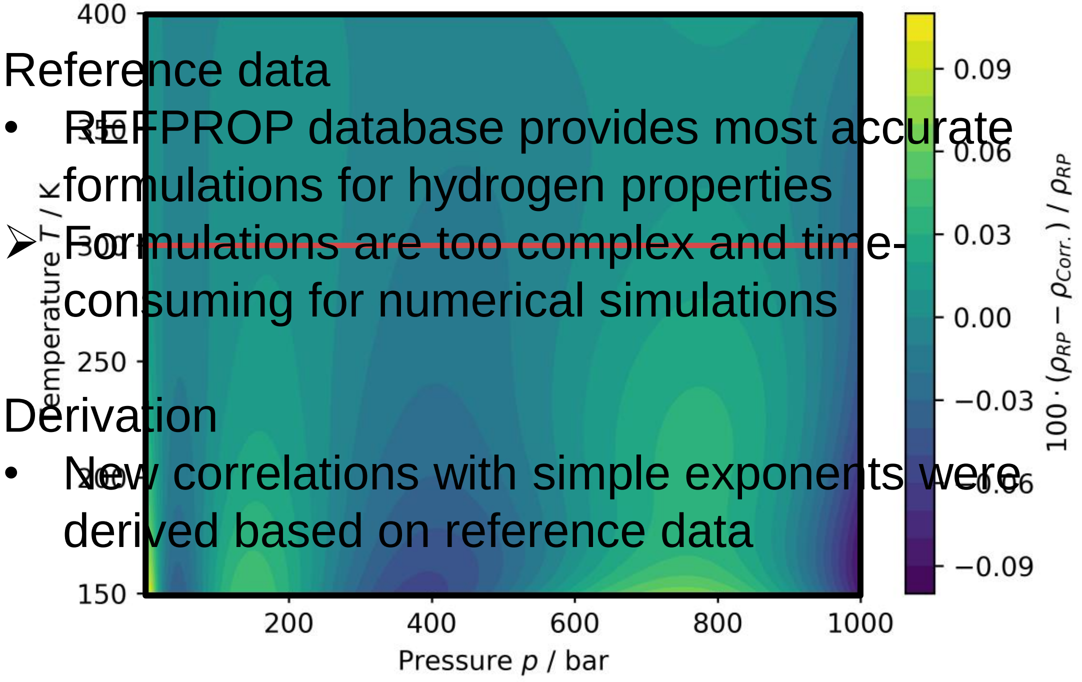
Reference data

- REFPROP database provides most accurate formulations for hydrogen properties

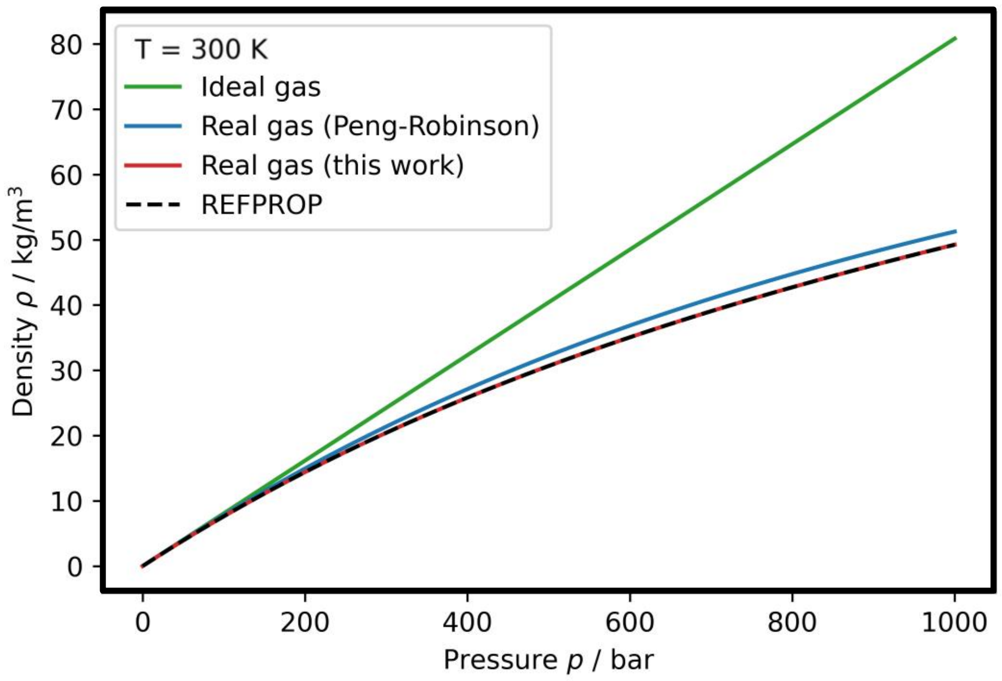
➢ Formulations are too complex and time-consuming for numerical simulations

Derivation

- New correlations with simple exponents were derived based on reference data



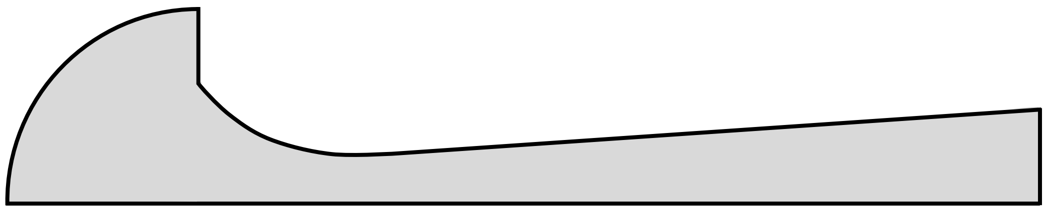
Hydrogen



➢ Error is decreased from 5 % (–) to 0.1 % (–)

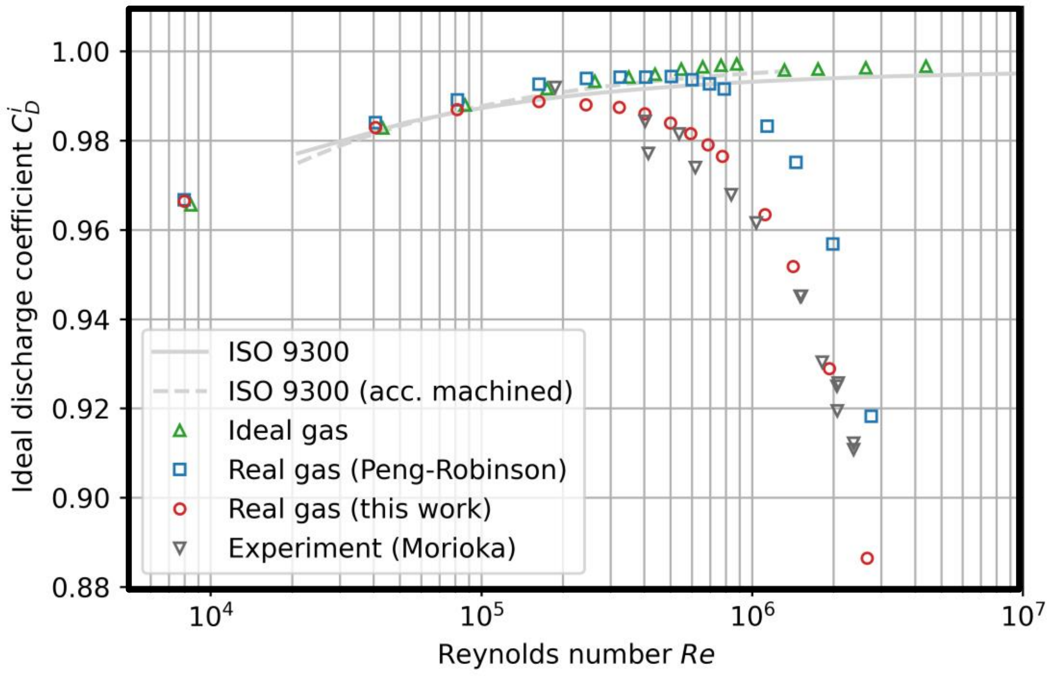
Real gas effects

Validation



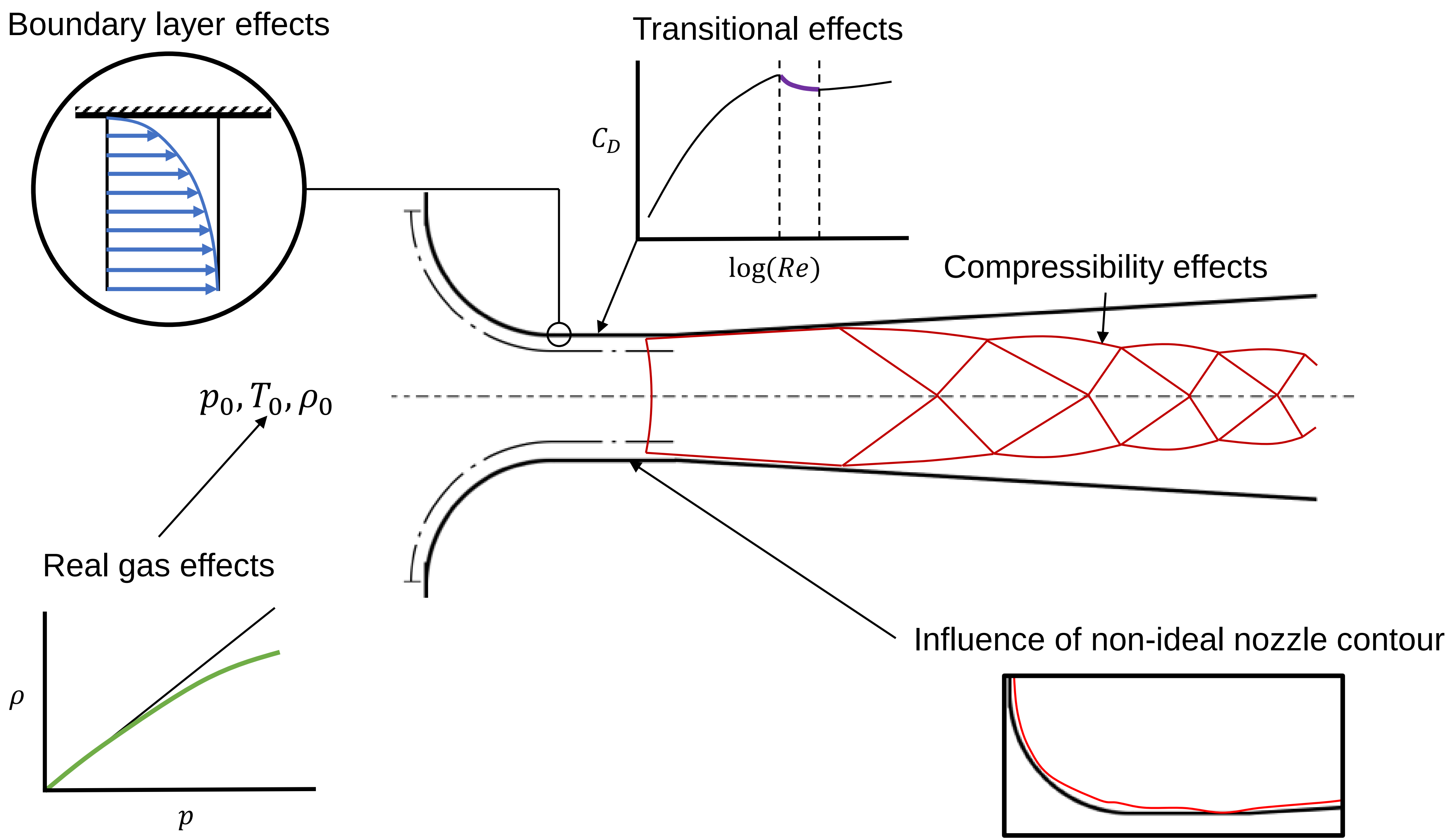
- Validation simulations of hydrogen nozzle flow with
  - △ Ideal gas model
  - □ Real gas model by Peng & Robinson
  - ○ Real gas model from this work
- compared with
  - ▽ Experiments by Morioka et al. (2011)

Toroidal nozzle (d = 0.6 mm, hydrogen flow)



➢ New implemented real gas model is in good accordance with experimental data

Non-ideal nozzle contours



Non-ideal nozzle contours

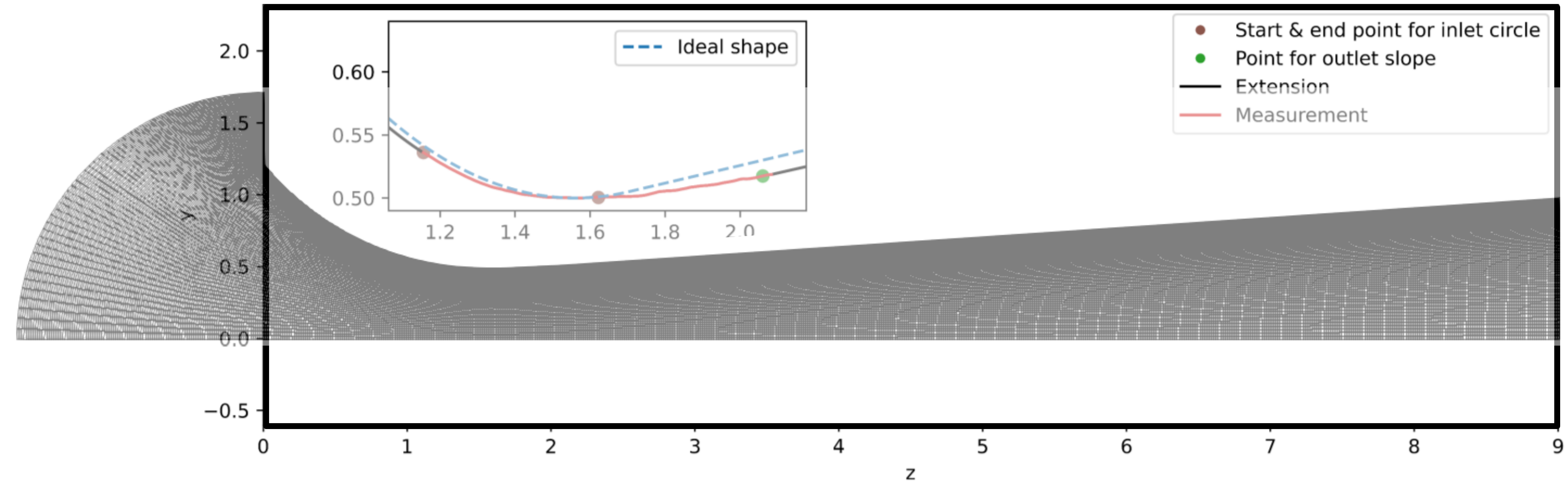
Geometry creation

- Measured nozzle contour (–) is extended (–) with
  - Circle at inlet
  - Straight line at outlet

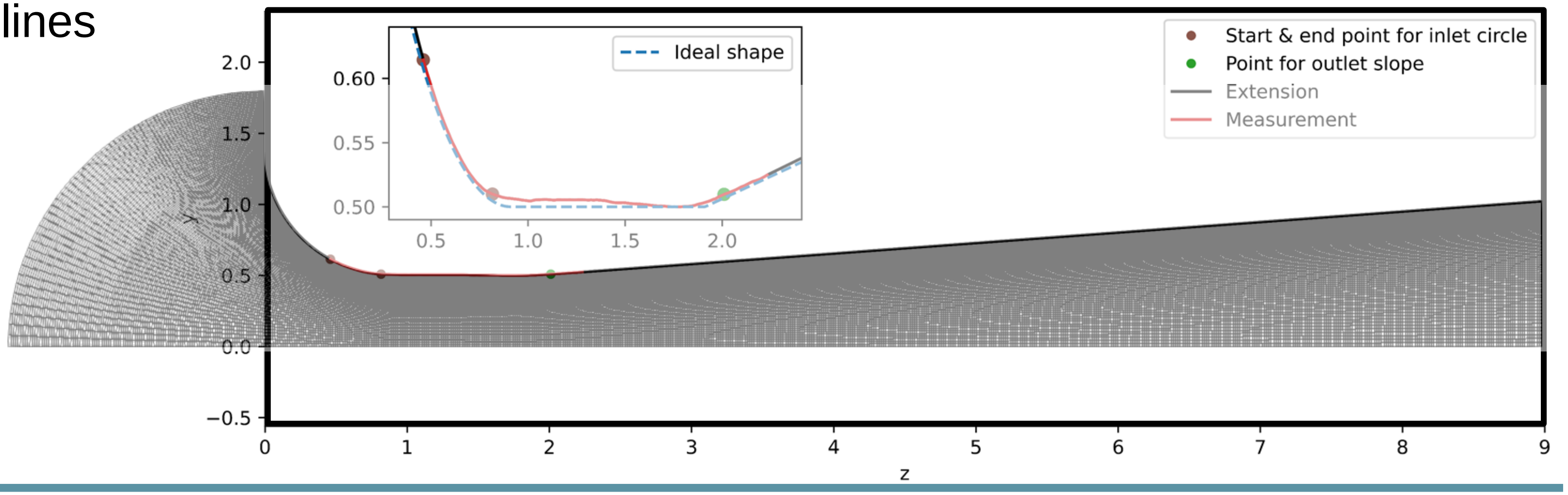
Mesh creation

- Hexaedral mesh
- Contour is implemented using B-splines
- Mesh can be created for
  - Ideal contours
  - Measured contours
  - Parameterized contours

Toroidal nozzle (d = 1 mm)



Cylindrical nozzle (d = 1 mm)

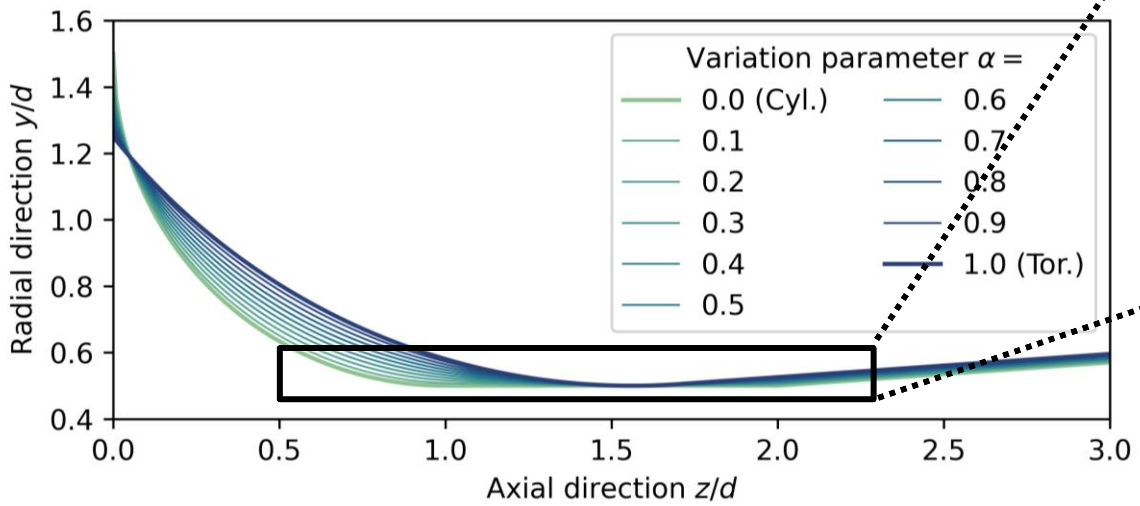


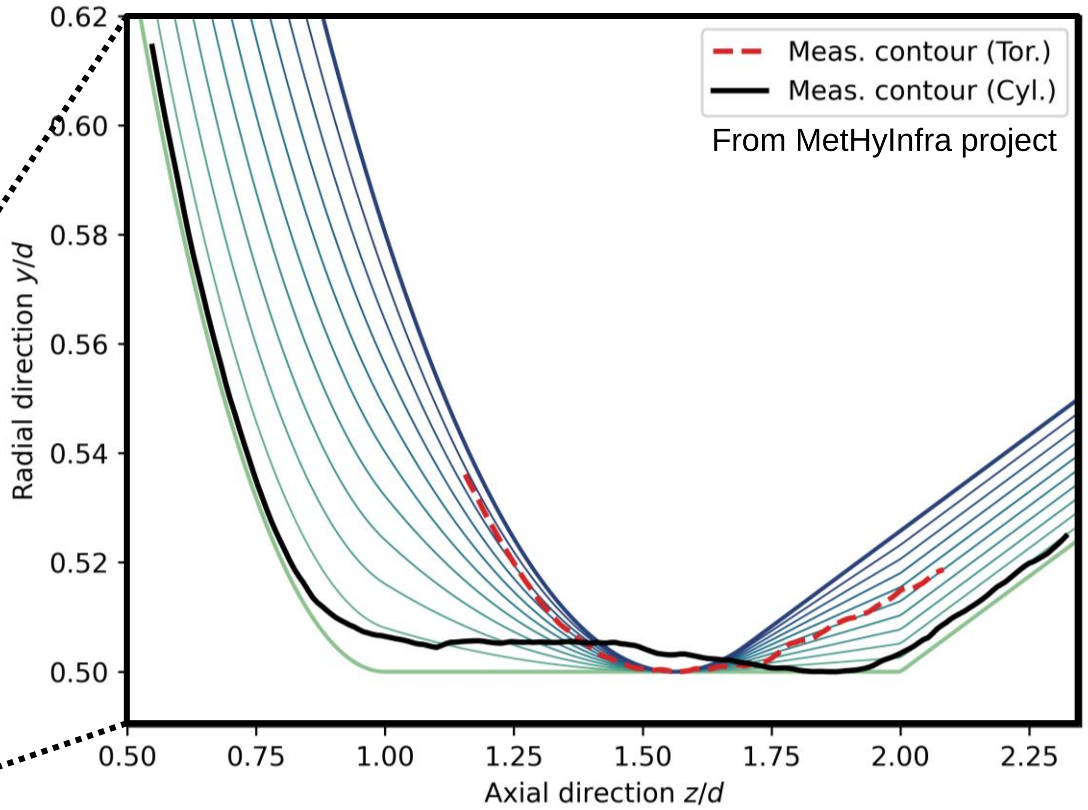
Parametric study

- Non-ideal nozzle shapes often lie between the two ideal shapes (cylindrical and toroidal)

➢ Let's consider a linear superposition of the ideal types via a variation parameter α with
  - $\alpha = 0$ for cylindrical shape
  - $\alpha = 1$ for toroidal nozzle shape
  - $0 < \alpha < 1$ for parametric shape

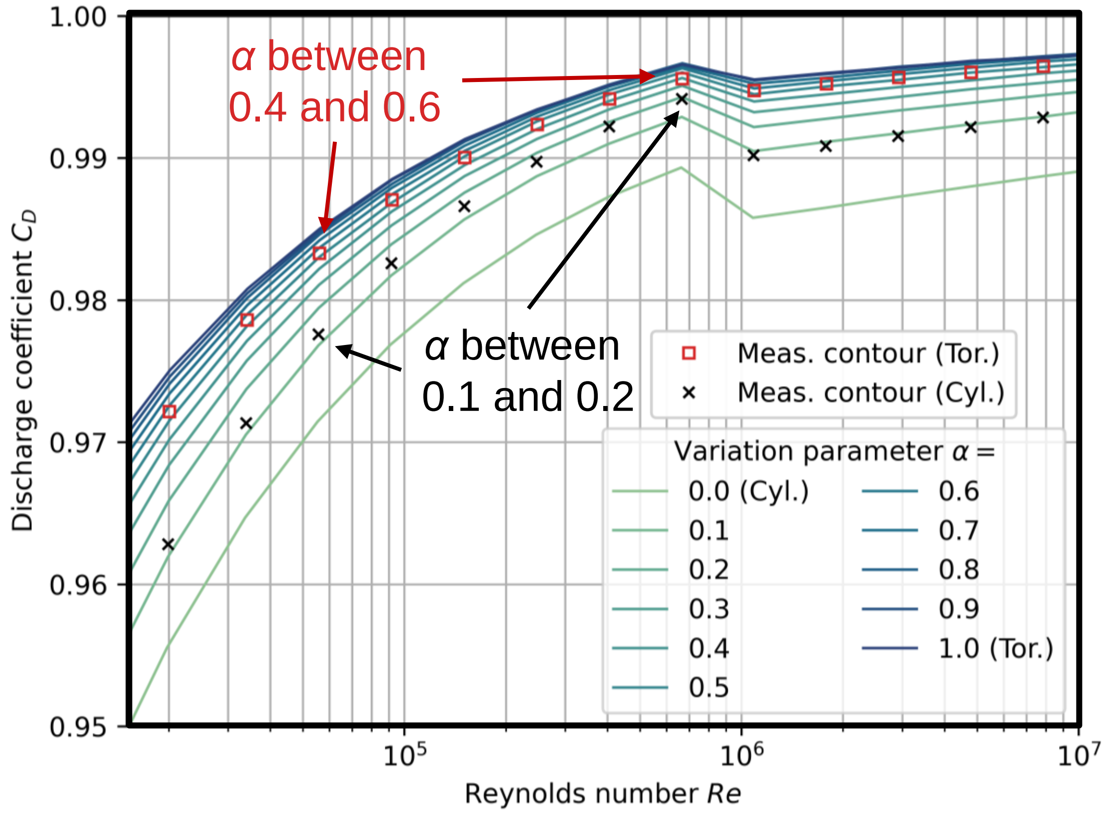
$$y(\alpha) = (1-\alpha)\cdot y_{Cyl} + \alpha \cdot y_{Tor}$$



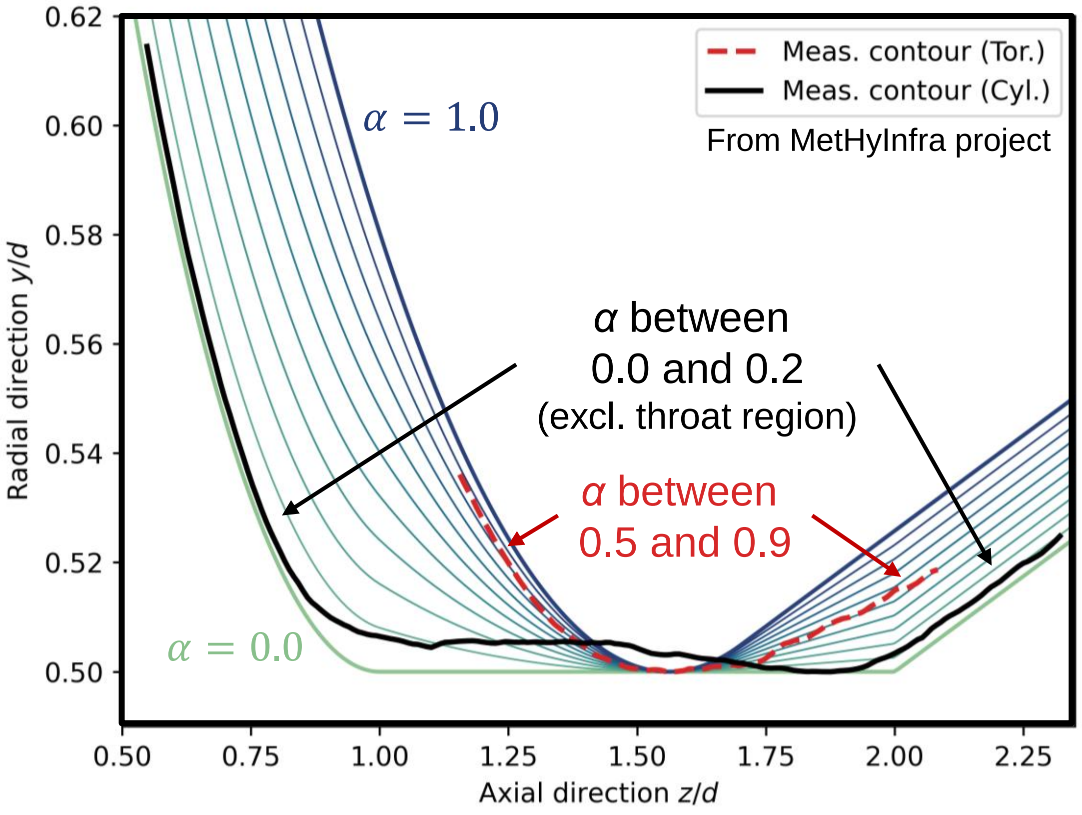


Parametric study

Results

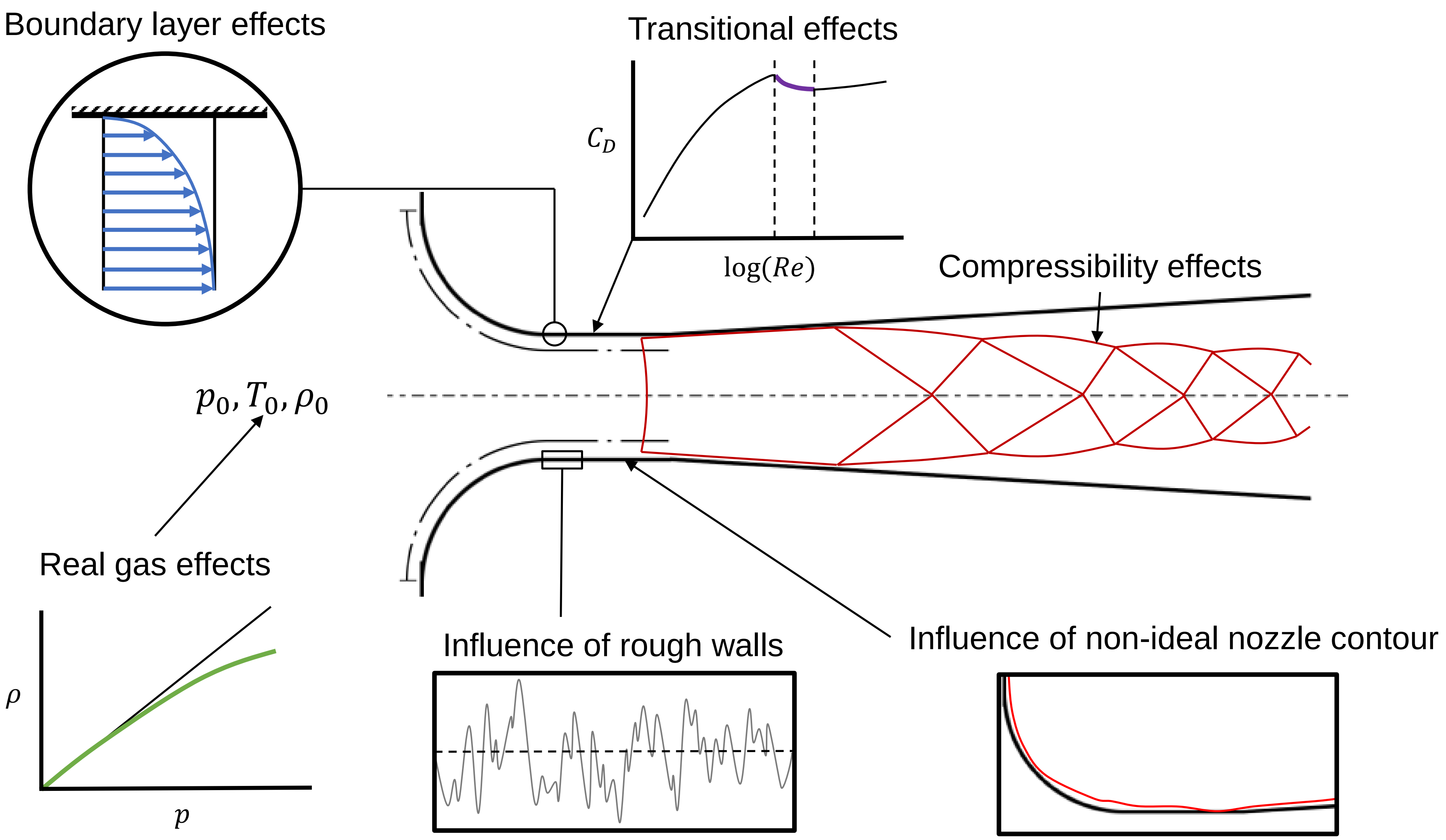


Nozzle contours



- ➢ In a first approximation, allocated α values of nozzle shapes coincide with those of the C_D curves

Wall roughness

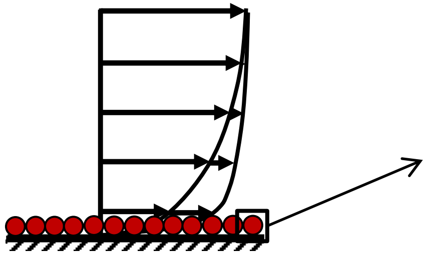


Wall roughness

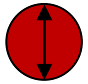
- Logarithmic law of the wall (smooth walls)

$$u^+ = \frac{1}{\kappa}\ln(Ey^+) \qquad 30 < y^+ < 200$$

- What happens for rough walls?



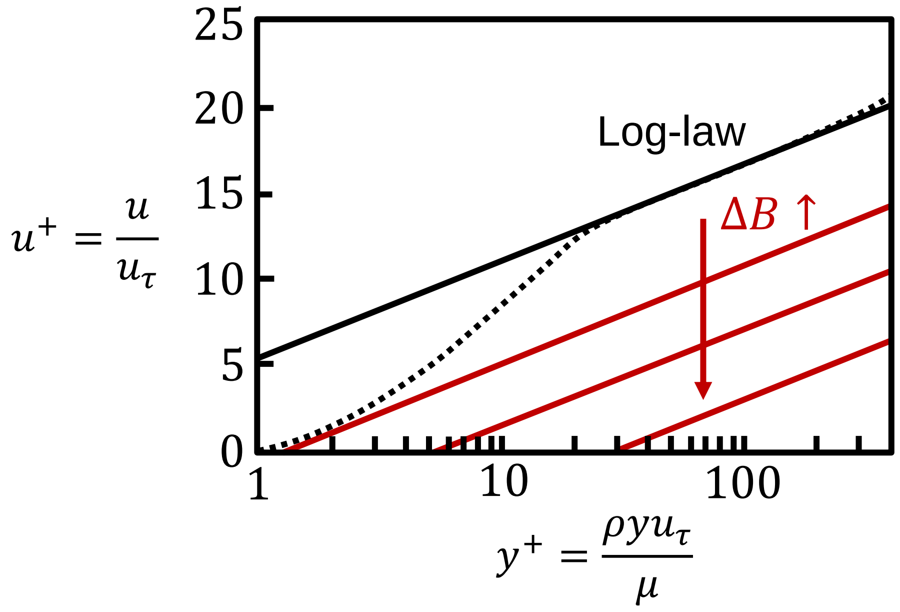
Sand grain roughness height

 K_s $\left(K_s^+ = \frac{\rho K_s u_\tau}{\mu}\right)$

- Sand grains increase wall shear stress and broaden the flow profile

➢ Logarithmic law of the wall (rough walls)

$$u^+ = \frac{1}{\kappa}\ln(Ey^+) - \Delta B$$



➢ ΔB causes the log-law curve to shift downwards

Three regions are distinguished

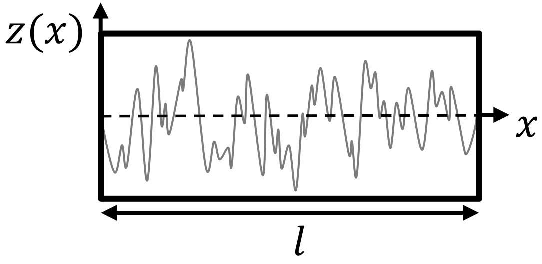
- Hydrodynamically smooth $K_s^+ \leq 2.25$
- Transitionally rough $2.25 < K_s^+ < 90$
- Hydrodynamically rough $90 \leq K_s^+$

Wall roughness

Roughness average *Ra*

- ➢ Arithmetic average of absolute values of profile heights over evaluation length

$$Ra = \frac{1}{l}\int_0^l |z(x)|\,dx$$

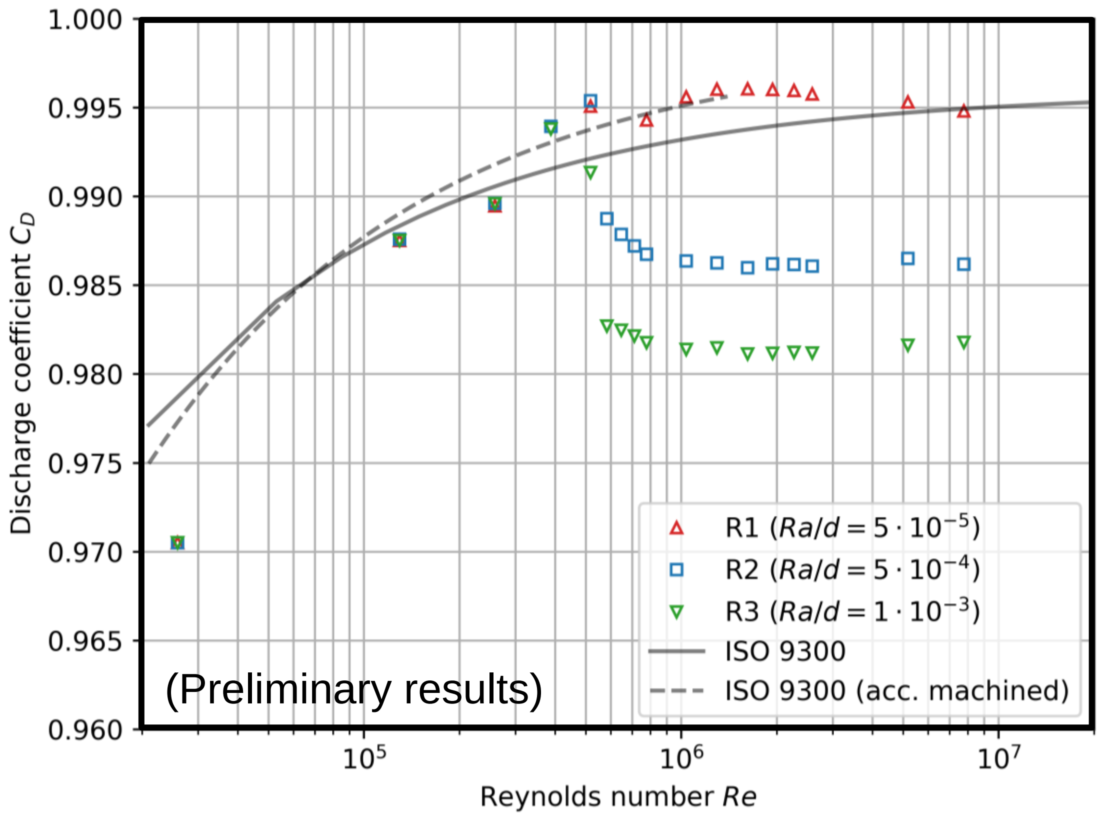


- Correlation between *Ra* and K_s for CFD analysis (based on literature study)

$$K_s \approx 5Ra$$

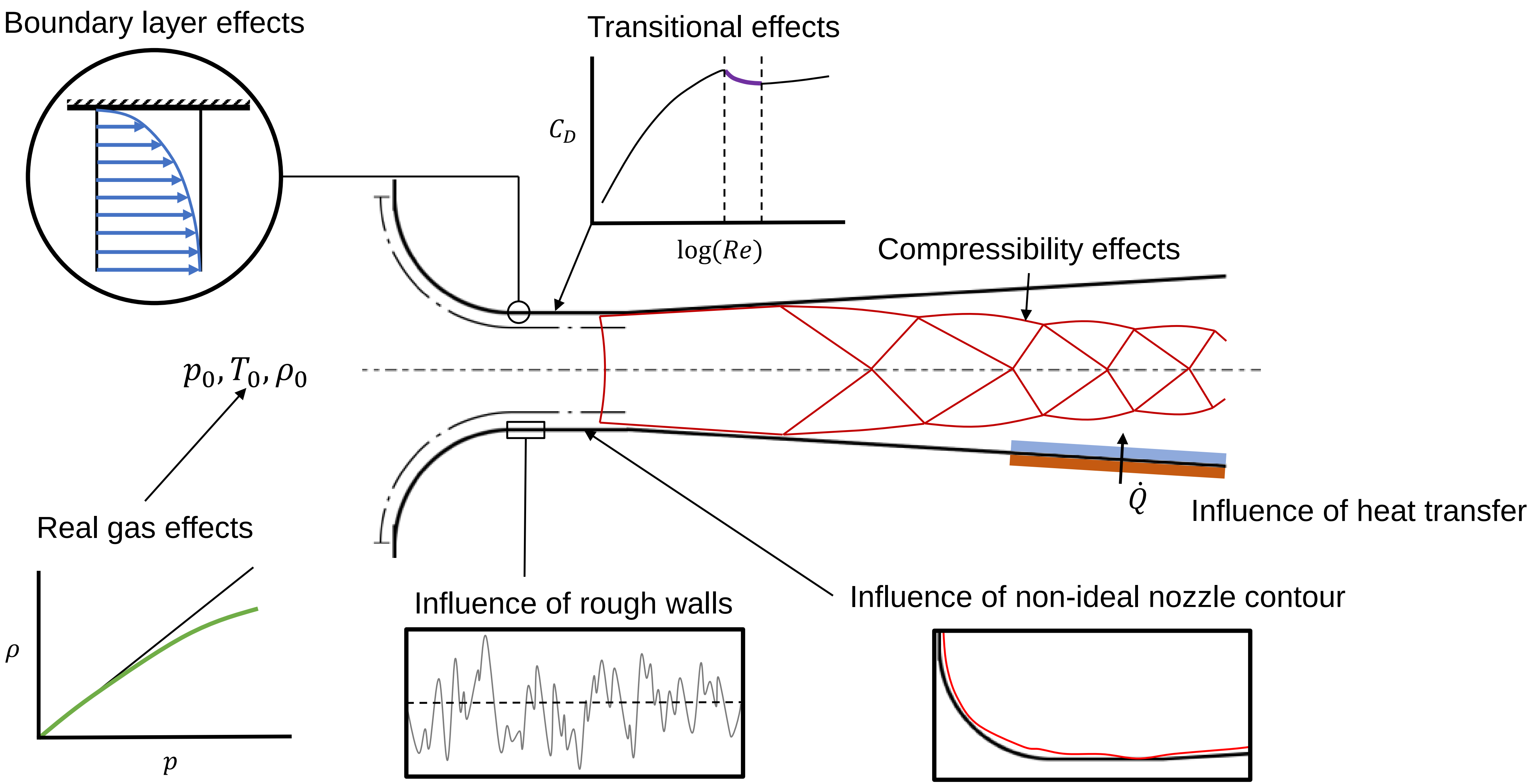
- Investigation of three different roughness levels:
  - △ R1 (*Ra* = 0.05 µm)
  - □ R2 (*Ra* = 0.50 µm)
  - ▽ R3 (*Ra* = 1.00 µm)

Toroidal nozzle
(d = 1.0 mm, hydrogen, ideal gas)



- ➢ Specific drop in turbulent region
- ➢ Transition occurs earlier

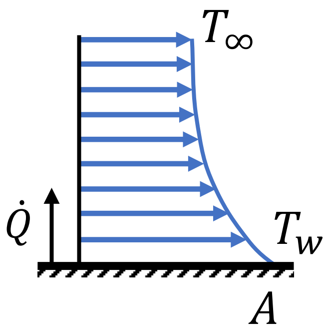
Heat transfer



Heat transfer

Thermal boundary layer (TBL)

- thin region close to wall formed due to temperature gradient between wall and core flow



Heat convection

$$\dot{Q} = hA(T_w - T_\infty)$$

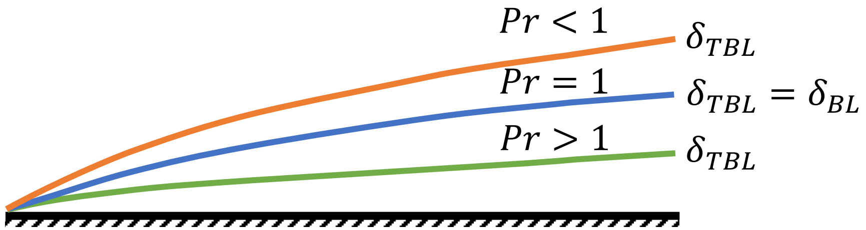
with heat transfer coefficient *h*

- As temperature in-/decreases in TBL, density de-/increases which affects mass flow rate $\left(\rho = \dfrac{p}{R_M T}\right)$

Prandtl number

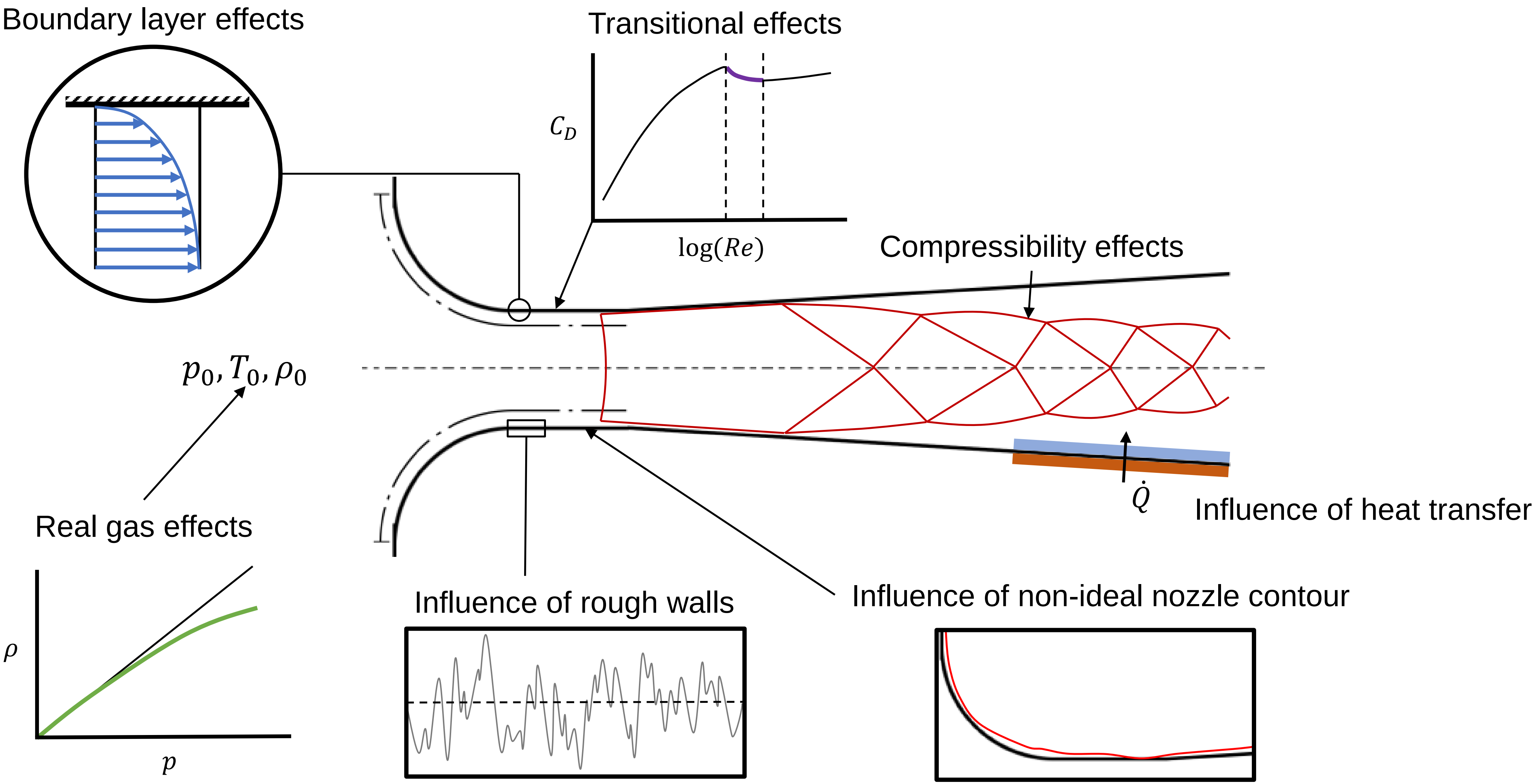
- Ratio of momentum to thermal diffusivity

$$Pr = \frac{\nu}{\alpha} = \frac{\mu/\rho}{k/(c_p\rho)} = \frac{c_p\mu}{k}$$



- For many gases, typically around 0.7

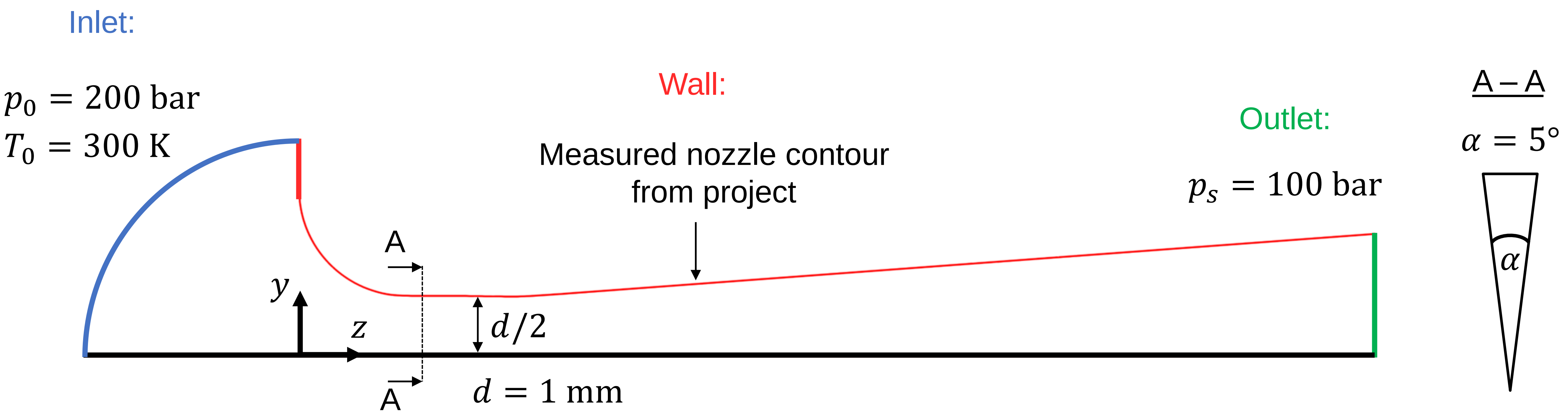
Thank you!



Boundary layer effects
Transitional effects
C_D
$\log(Re)$
Compressibility effects
p_0, T_0, ρ_0
$\dot{Q}$
Influence of heat transfer
Real gas effects
ρ
p
Influence of rough walls
Influence of non-ideal nozzle contour

Next session: Tutorial case

High-pressure hydrogen flow through a cylindrical non-ideal critical nozzle



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MetHyInfra

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