

um  
2026

# Reduced Order Modeling of Tubular Reactors for Synthetic Methane Production

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# Motivation

## Why Tubular Reactors?

🏭 Large-scale production of base chemicals (methane, methanol, ethane)

⚙️ High throughput and industrial reliability

🔄 Continuous operation

## Challenges

🌡️ Heat transfer and temperature control

🚫 Catalyst deactivation over time

🔧 Clogging and pressure drop

## Why Synthetic Methane?

♻️ Enables Power-to-X pathways

⚡ Converts renewable electricity into chemical energy

🟢 Supports green hydrogen utilization



Image Sources: Everllence ([www.everllence.com](http://www.everllence.com)); IFA Technology ([www.ifa-technology.net](http://www.ifa-technology.net))

# Agenda

Objectives

Methodology

Results & Discussions

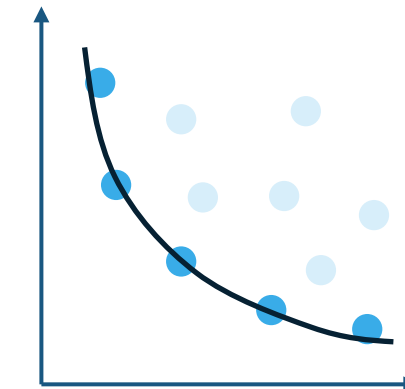
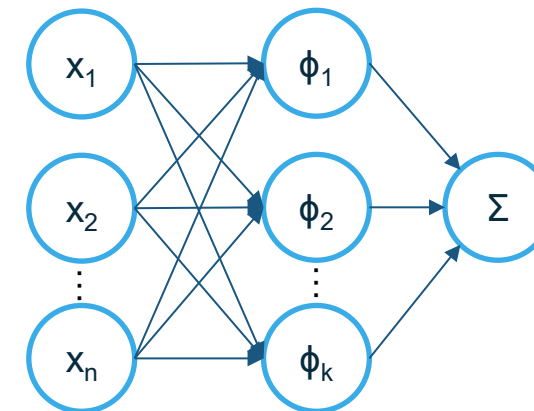
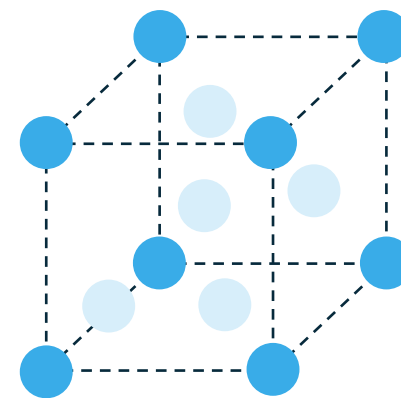
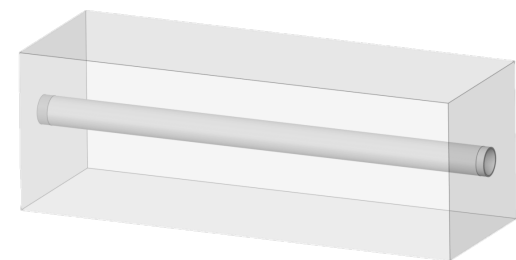
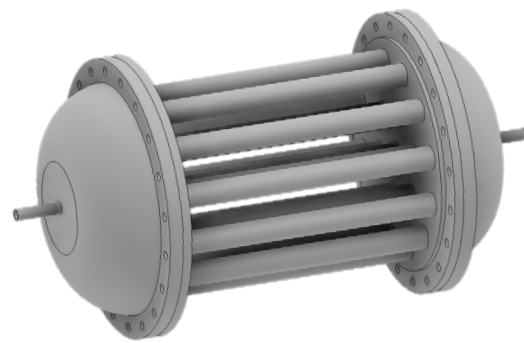
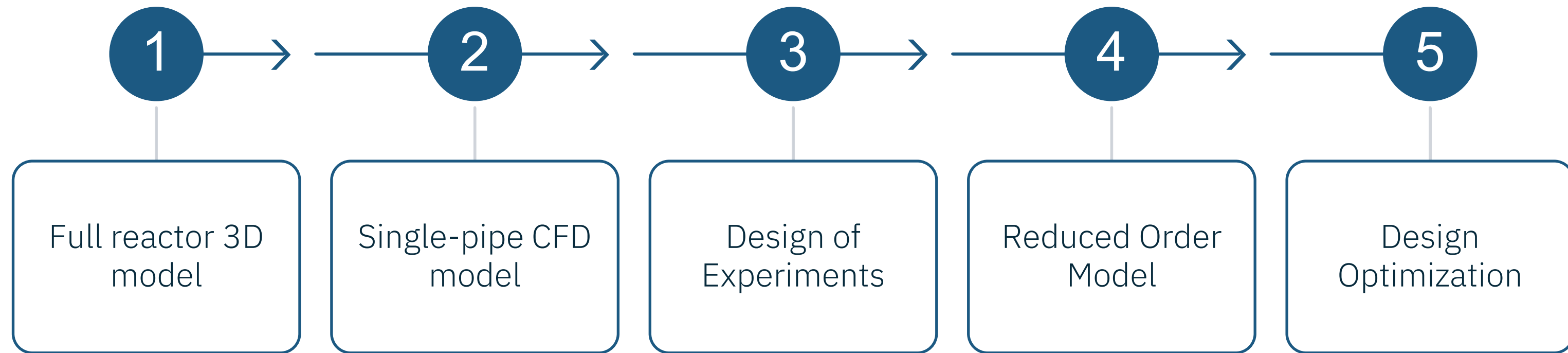
Conclusions & Outlook



# Objectives



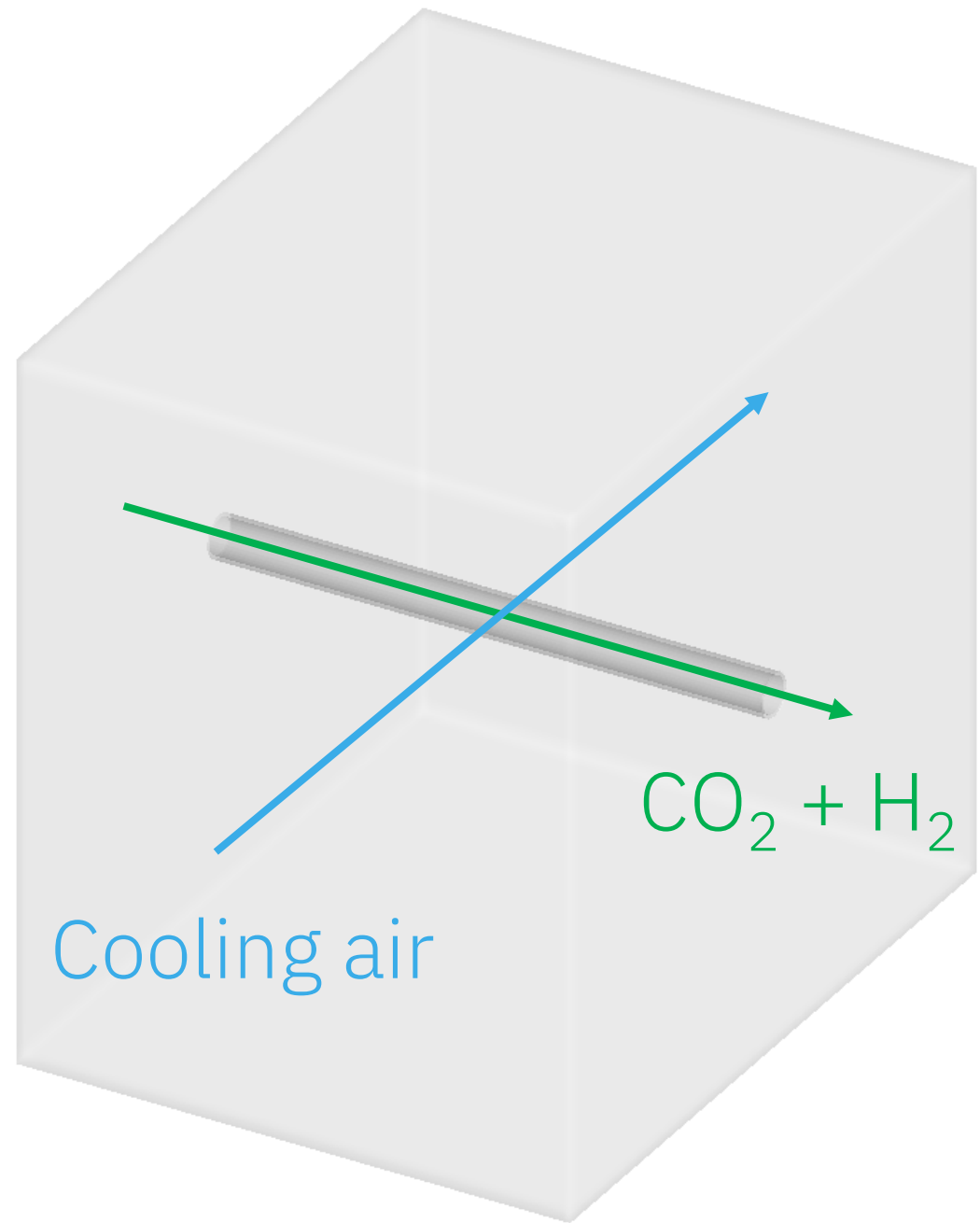
# Develop workflow to optimize chemical tubular reactors



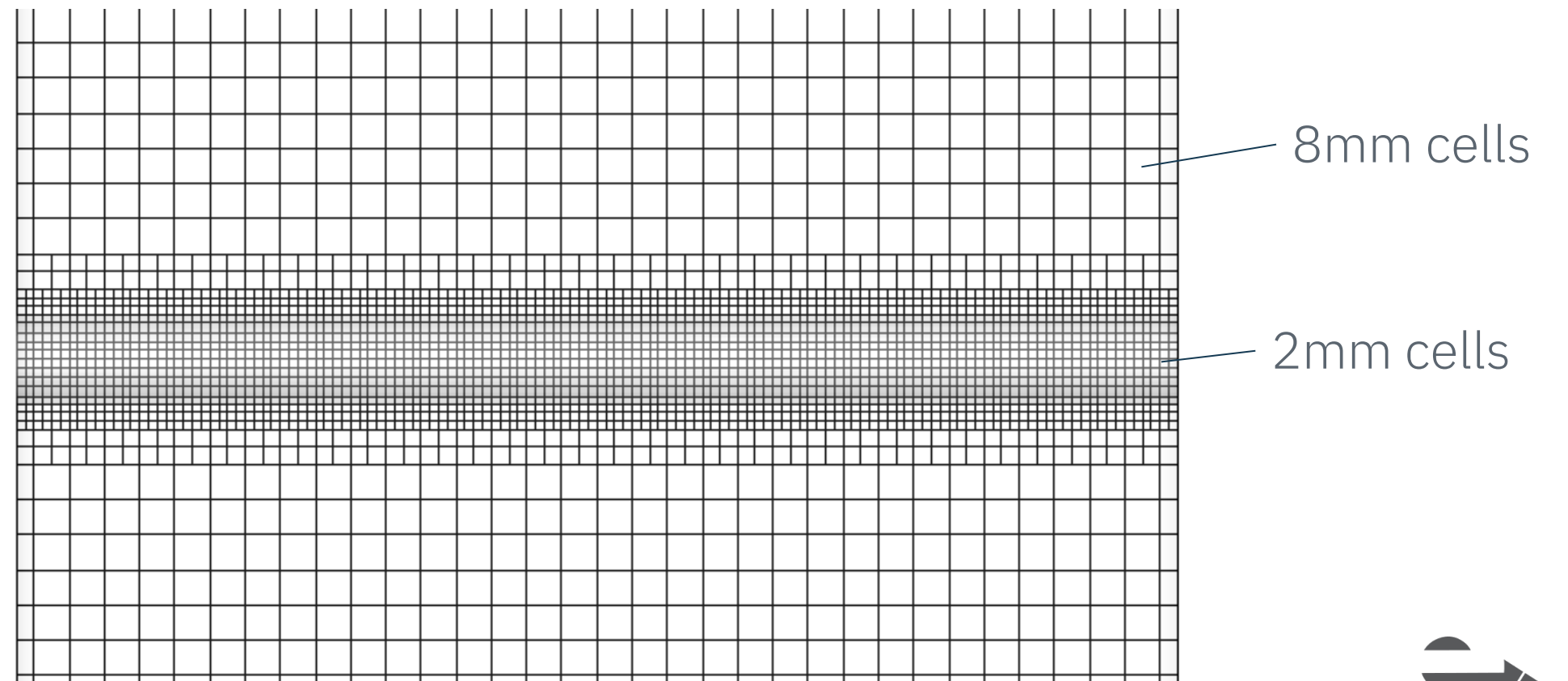
# Methodology



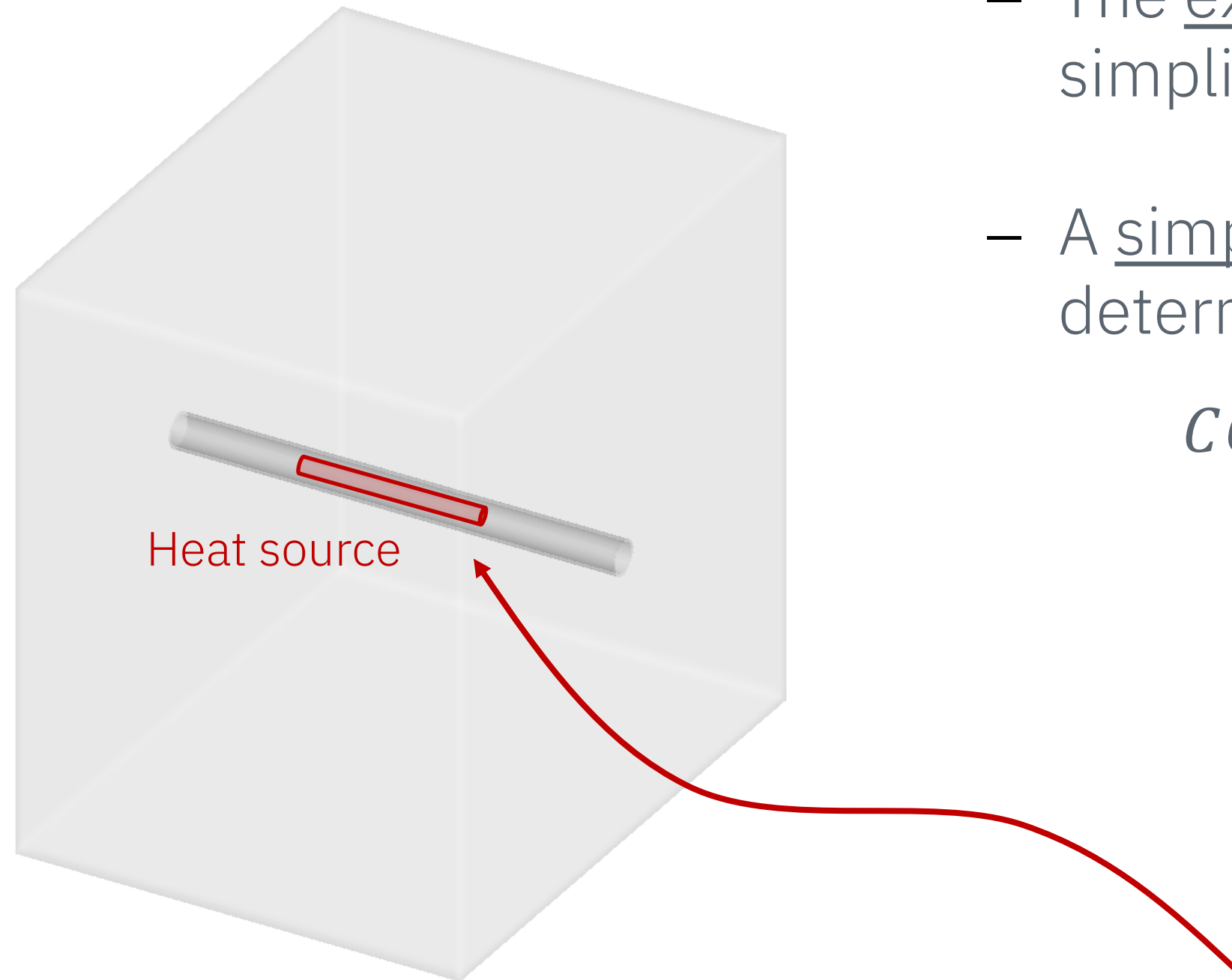
# 3D-CFD tubular reactor model



- Single-pipe geometry surrounded by flow box
- Flow and conjugate heat transfer simulation performed in Converge CFD v3.1.8
- Fixed mesh embedding at pipe walls



# 3D-CFD tubular reactor model



- The exothermic CO<sub>2</sub> methanation reaction is simplified by a heat source
- A simple one-step reaction is used to determine the heat power



$$R = r \cdot V_{reaction} \quad \text{Eq. 2}$$

$$r = k \cdot [CO_2][H_2] \quad \text{Eq. 3}$$

$$k = A \cdot \exp\left(-\frac{E_a}{RT}\right) \quad \text{Eq. 4}$$

$$\dot{Q} = -1 \cdot \underbrace{\Delta_R H}_{\text{Reaction enthalpy}} \cdot R \quad \text{Eq. 5}$$

# Reduced Order Model

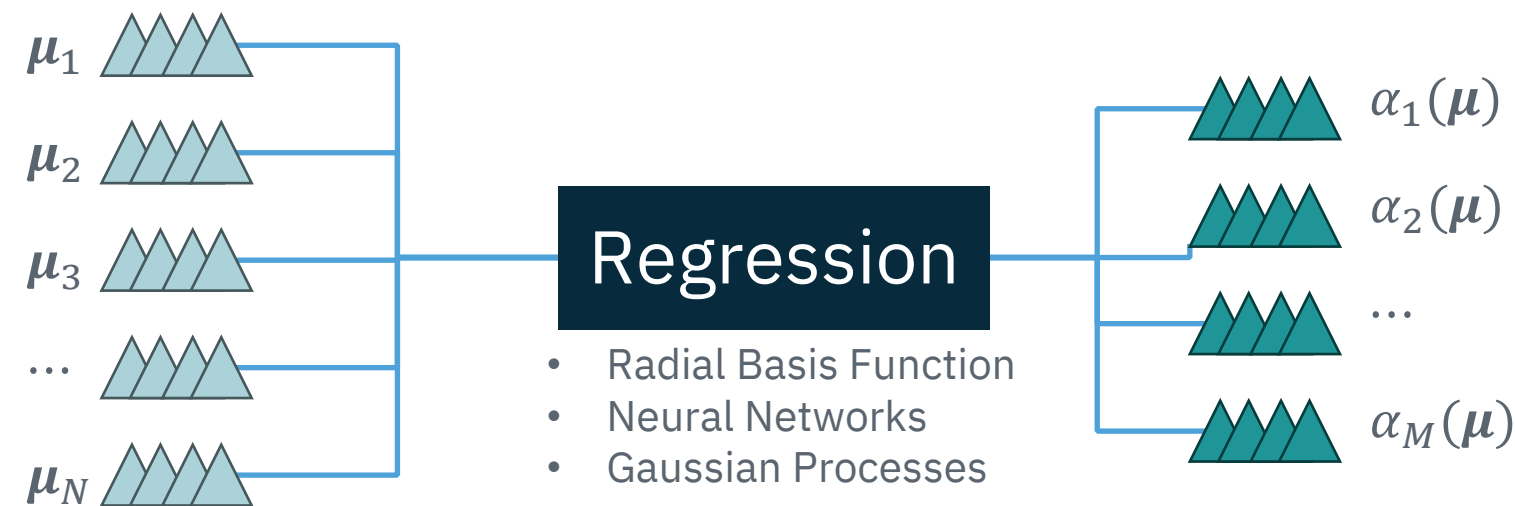
## Training

For a set of given solution snapshots,  $y = [y_1, y_2, \dots, y_N] \in \mathbb{R}^{n \times N}$  with  $y_i = y_i(\mu_i)$ , where  $\mu_i$  is the parametrization of the input space,

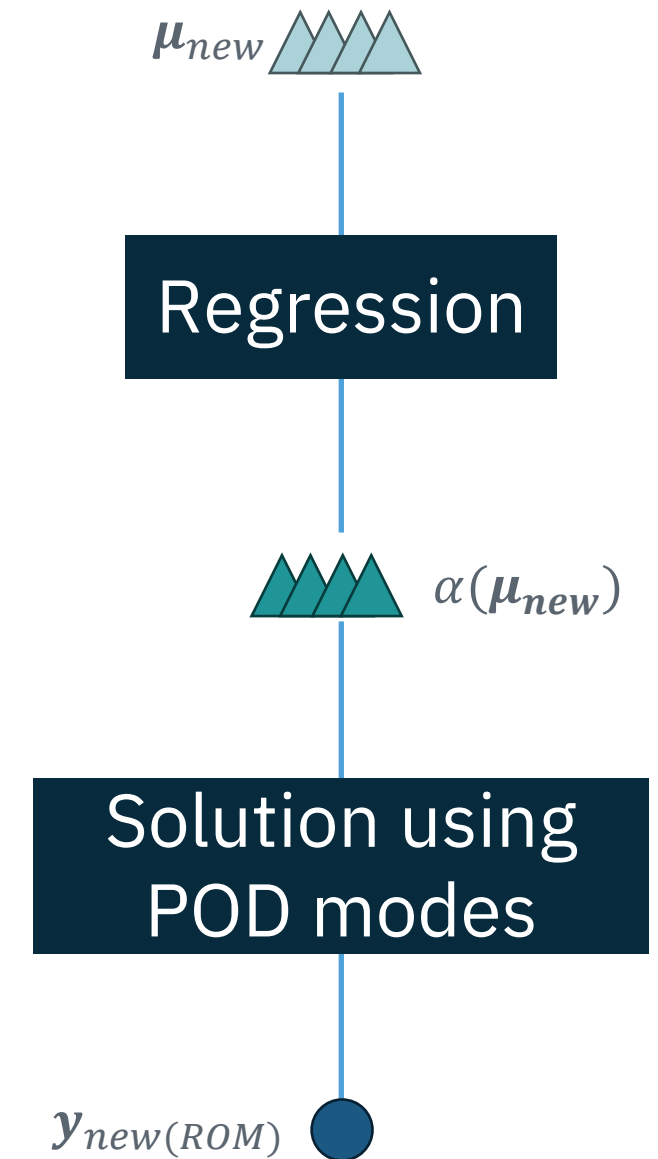


$$y_{ROM} = \sum_{i=1}^M \alpha_i \psi_i \text{ for } i = 1, \dots, M$$

Where M determines the level of information compression at the cost of model accuracy.



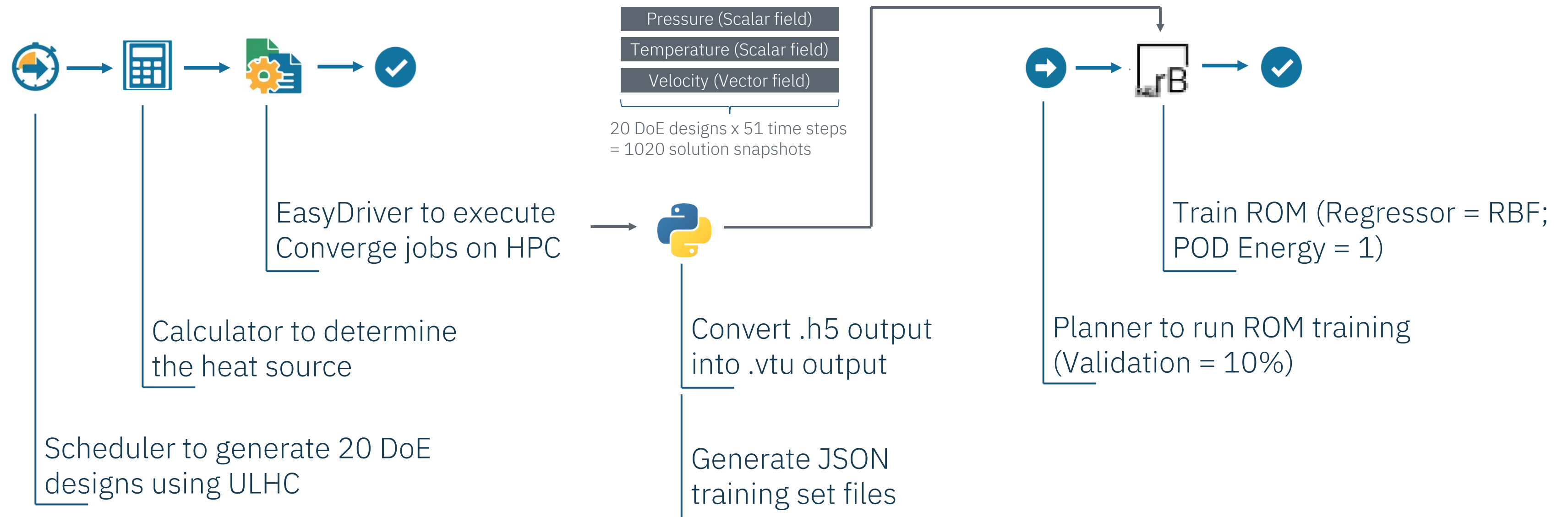
## Prediction



Graphic courtesy: OPTIMAD

# Converge CFD and ROMbox simulation workflow

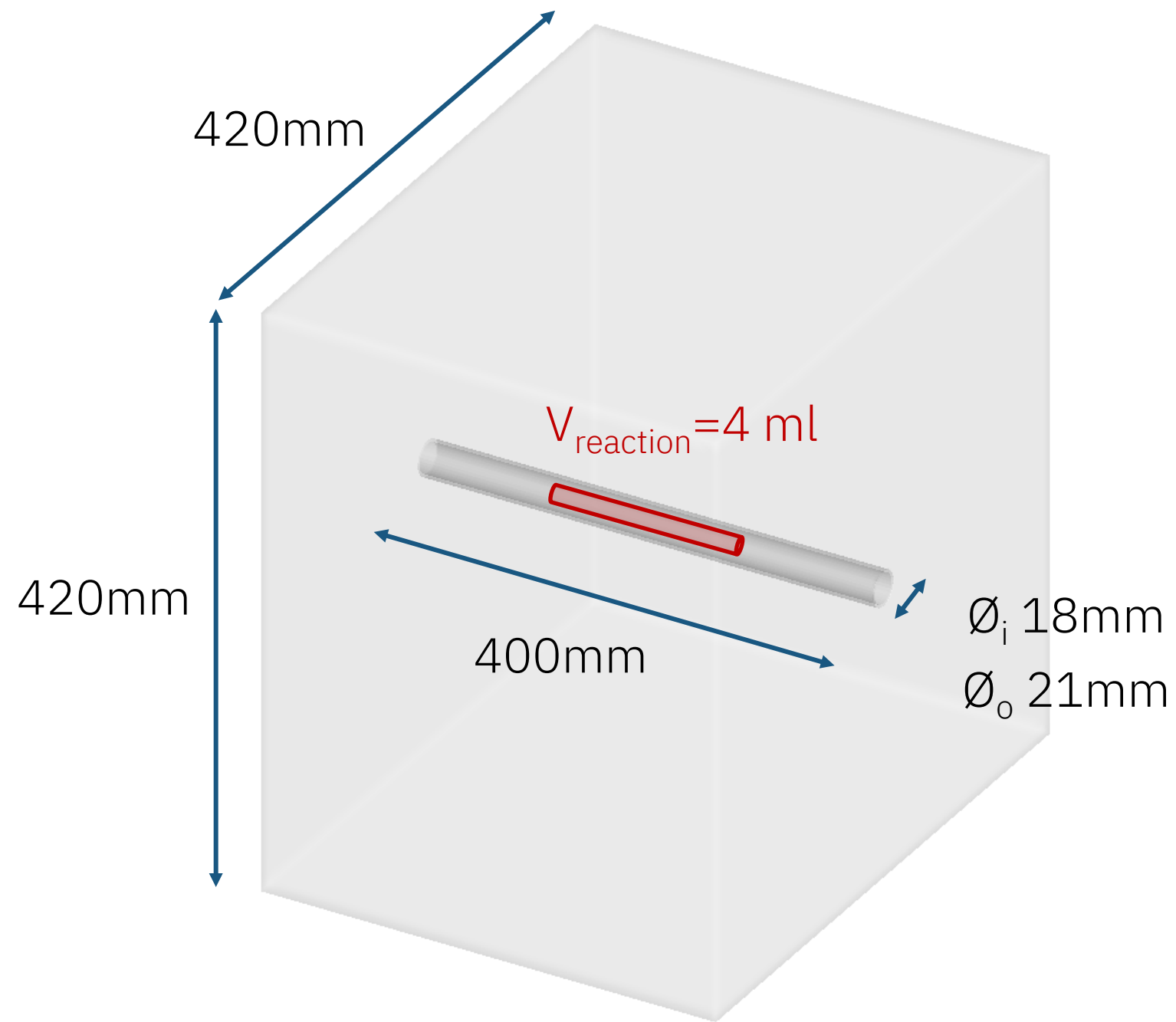
- Two modeFRONTIER 2025R2 workflows are developed to generate the ROM



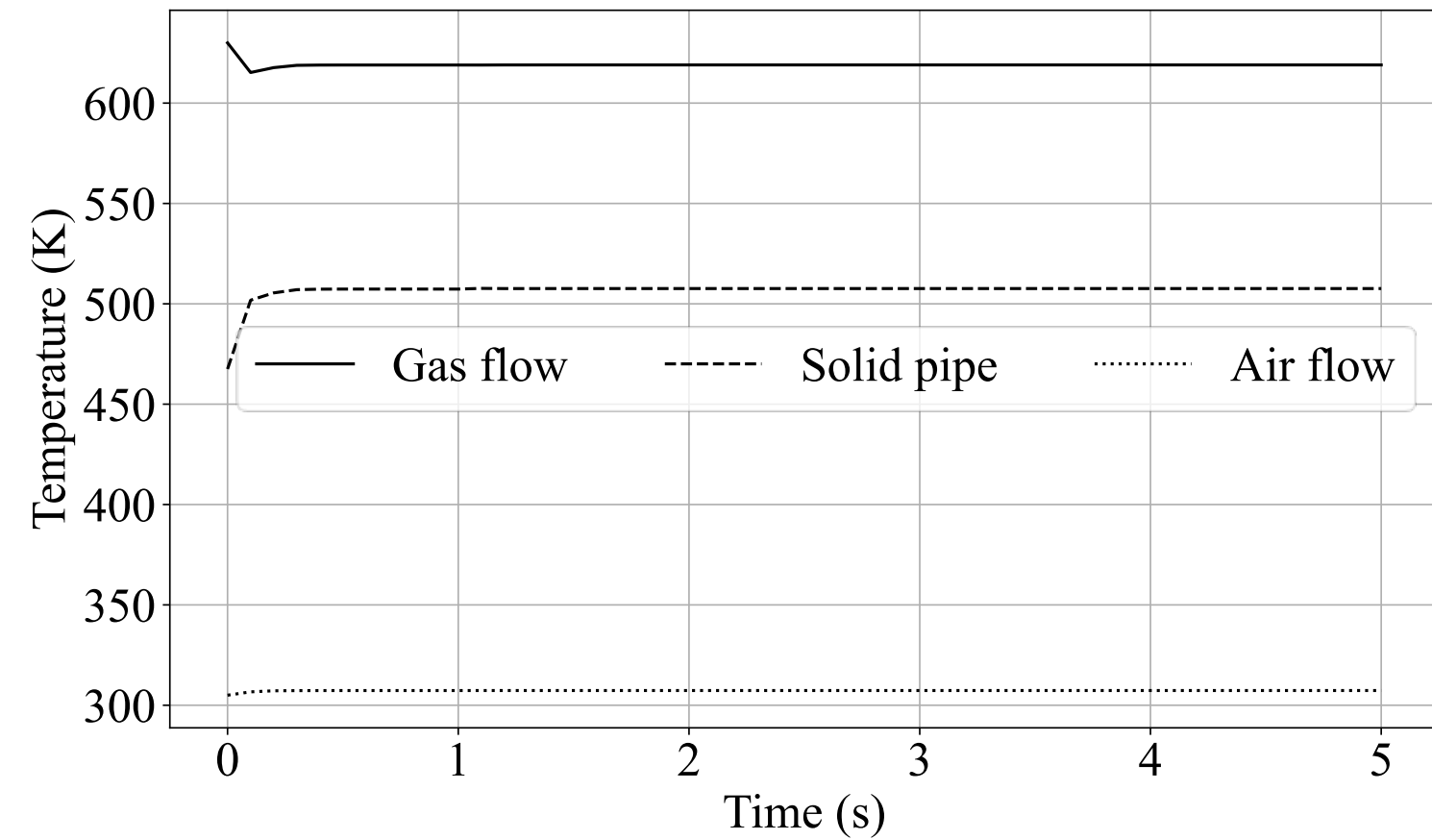
# Numerical Test Case



# CFD model setup



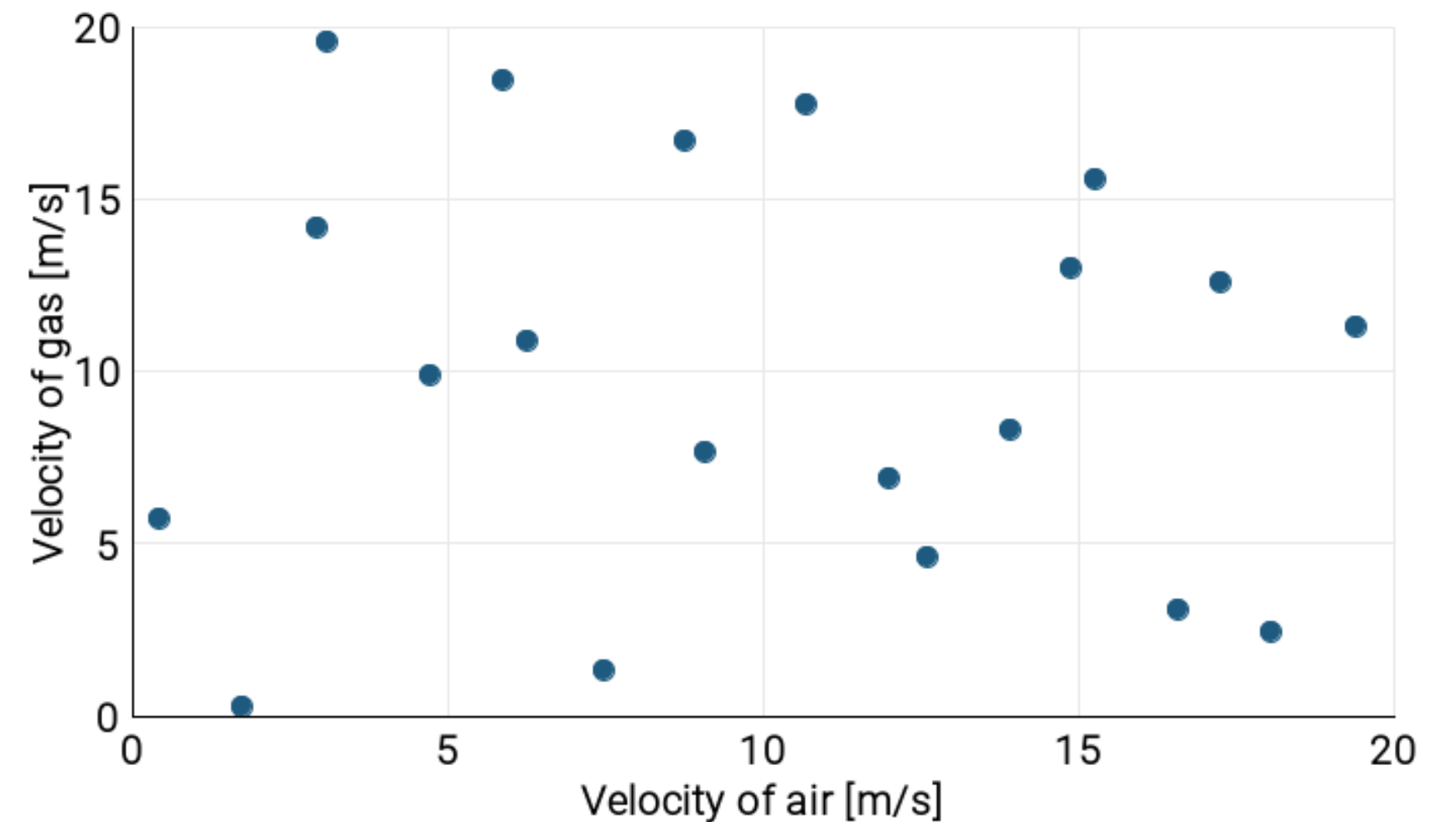
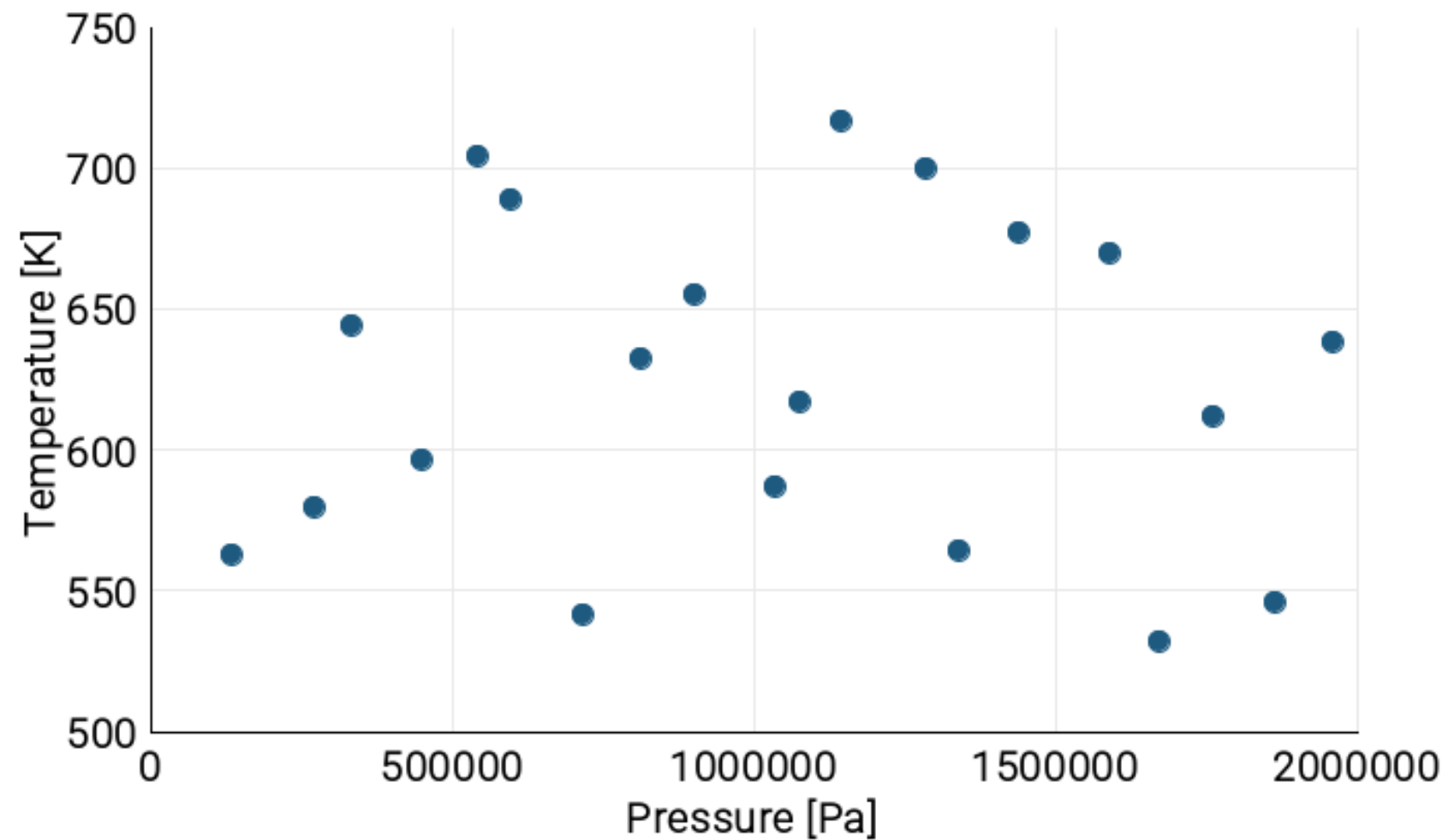
Example of a calculated temperature profile



- Simulation final time is set to 5 seconds
- Super cycling solves conjugate heat transfer every 0.05 seconds
- Heat source is activated at 0.01 seconds

# Design of Experiments

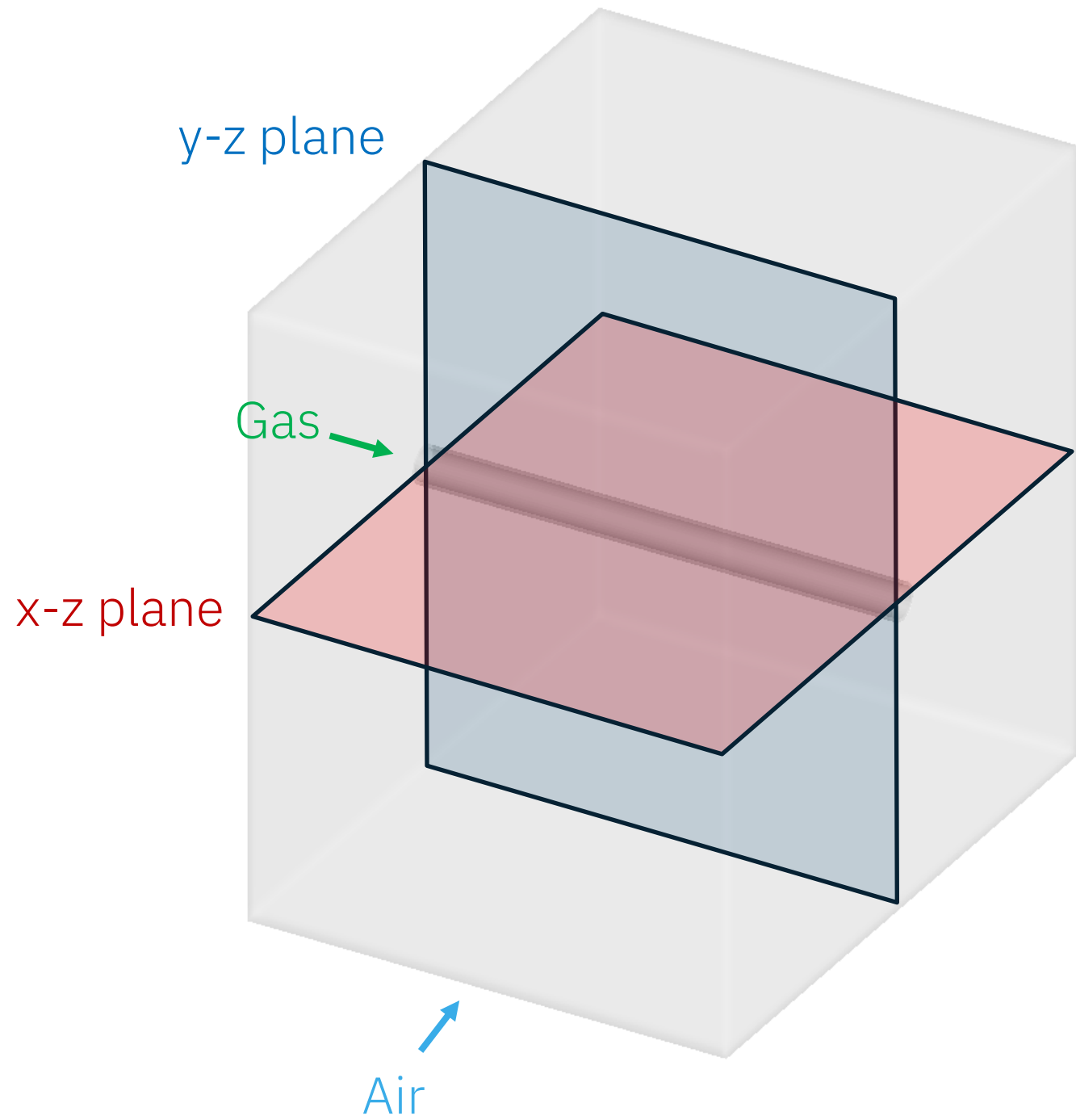
- 20 DoE points are generated using the Uniform Latin Hypercube algorithm



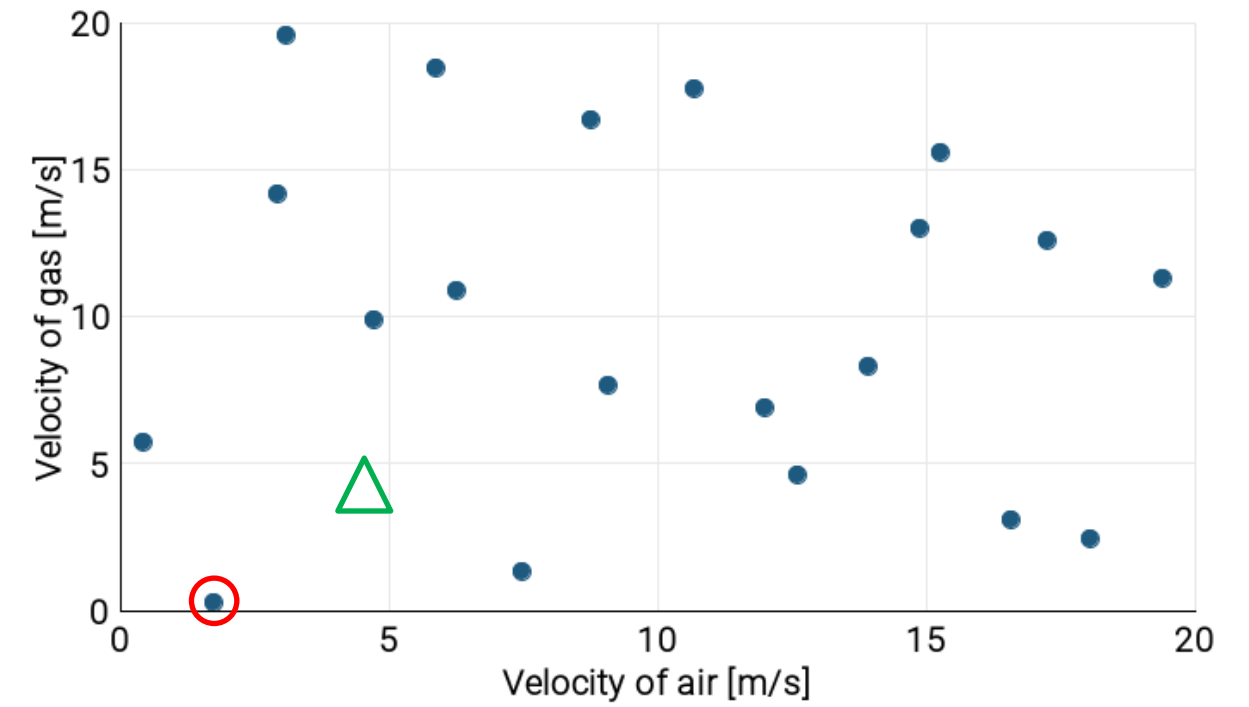
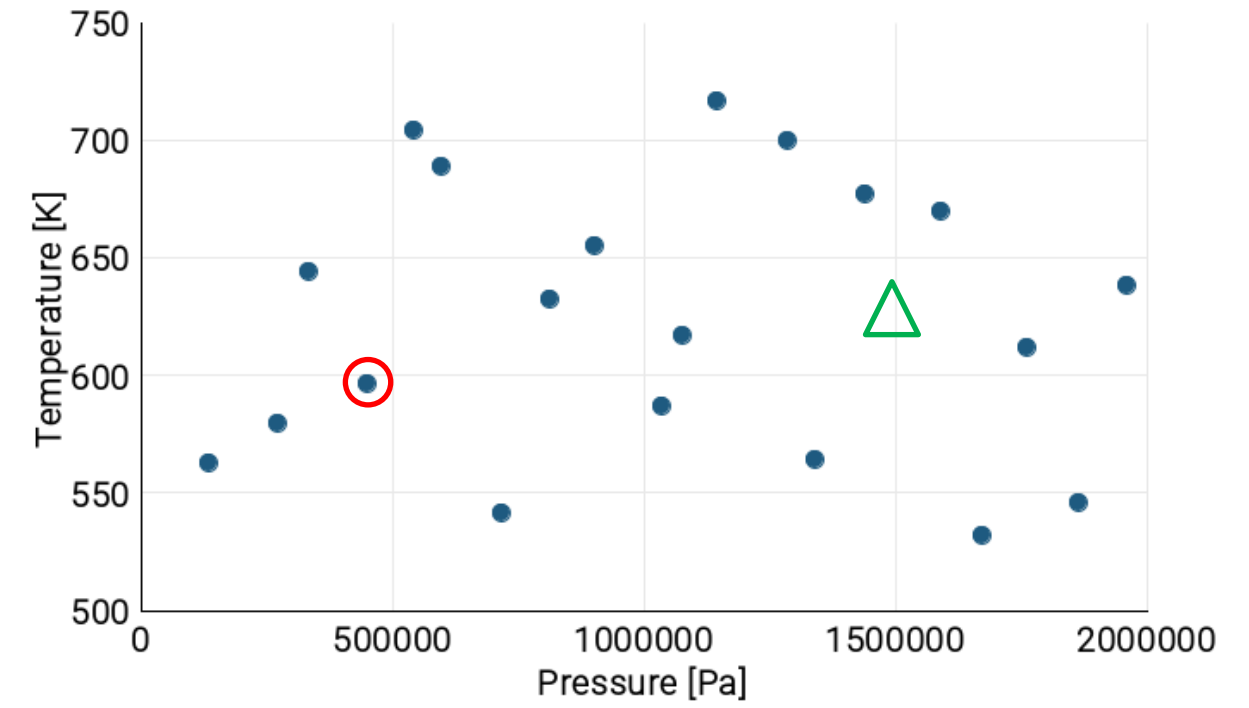
# Results & Discussion



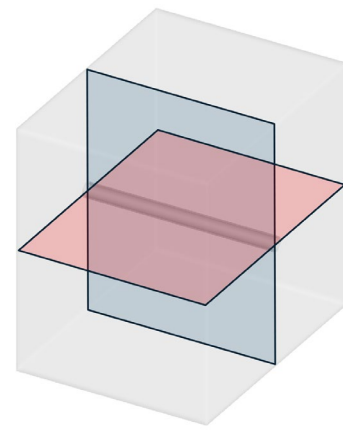
# Views and evaluation cases



- Compare Original and Prediction
- △ New Design

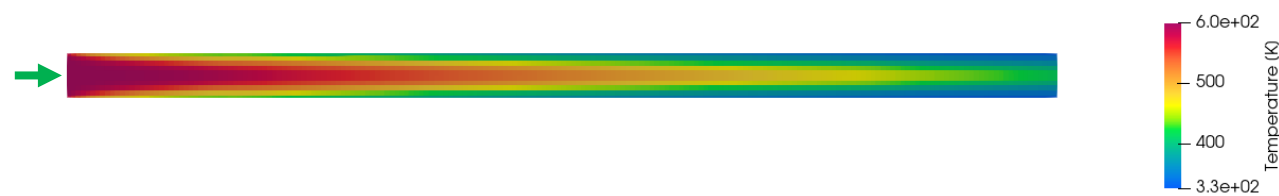


# Temperature of original solution and prediction

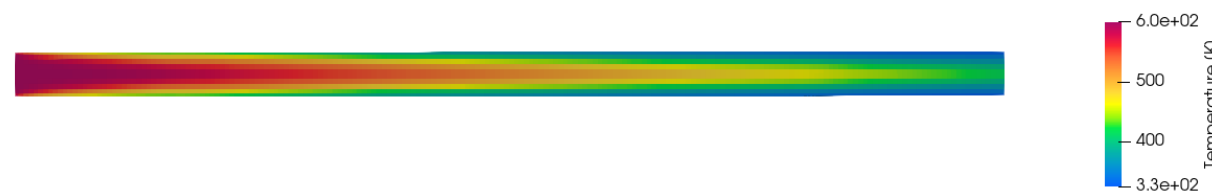


Gas flow  
(y-z)

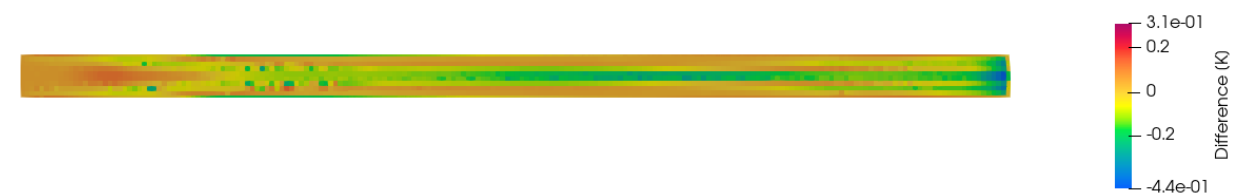
Original (y-z plane)



Prediction (y-z plane)

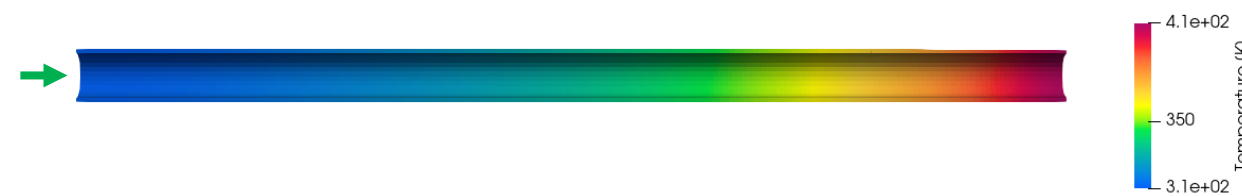


Difference (y-z plane)

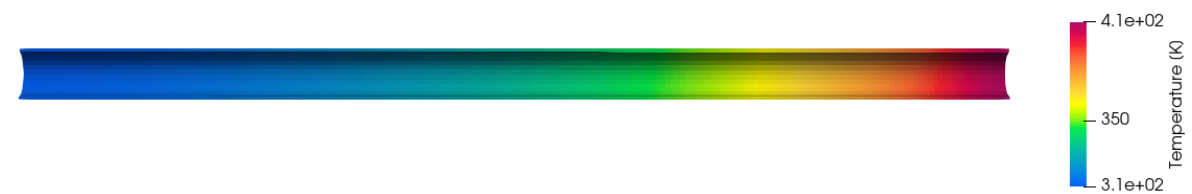


Solid pipe  
(x-z)

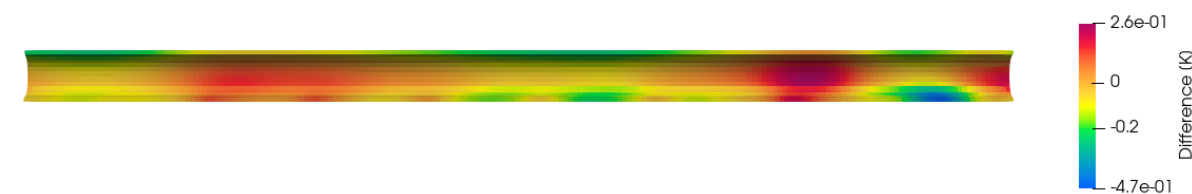
Original (x-z plane)



Prediction (x-z plane)

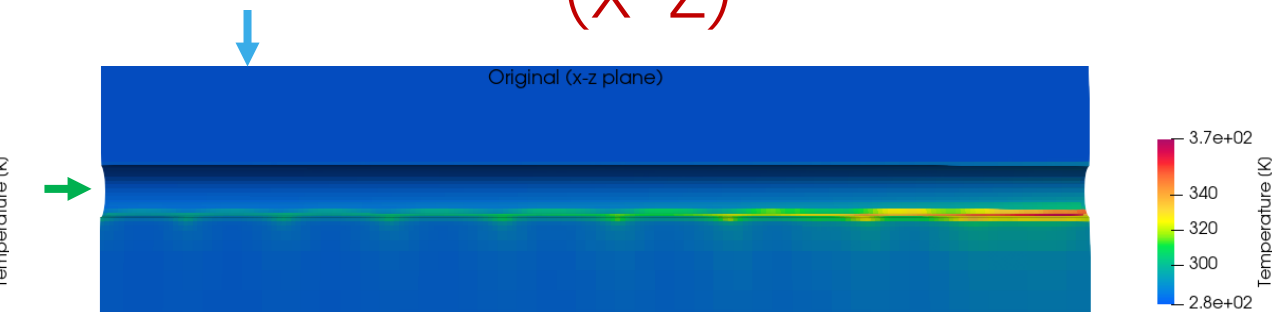


Difference (x-z plane)



Air flow  
(x-z)

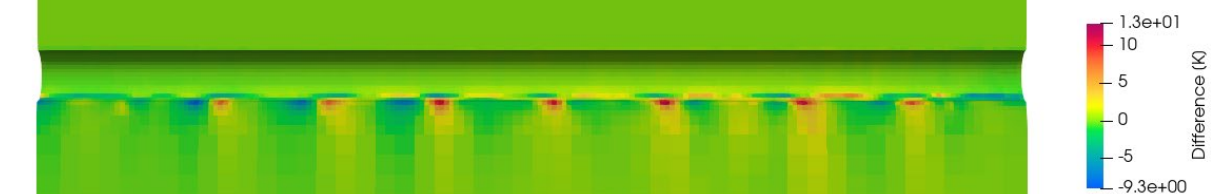
Original (x-z plane)



Prediction (x-z plane)

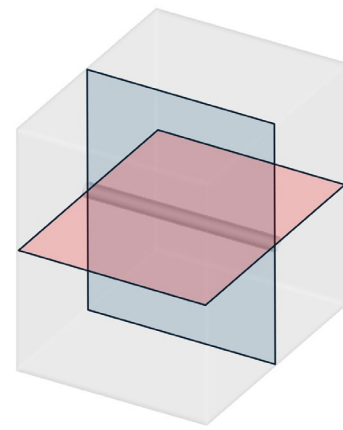


Difference (x-z plane)



– For temperature, the prediction shows a good agreement with the original solution

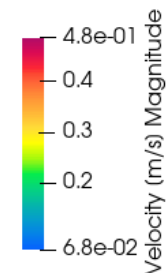
# Velocity of original solution and prediction



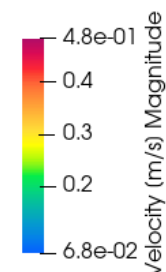
Gas flow

(y-z)

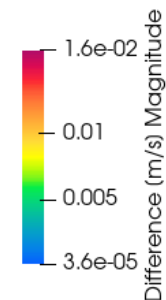
Original (y-z plane)



Prediction (y-z plane)



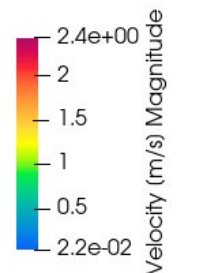
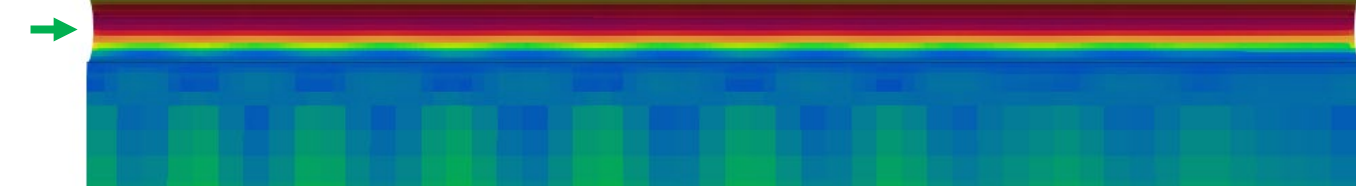
Difference (y-z plane)



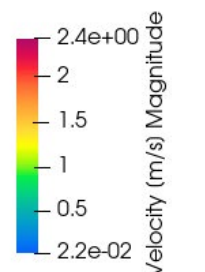
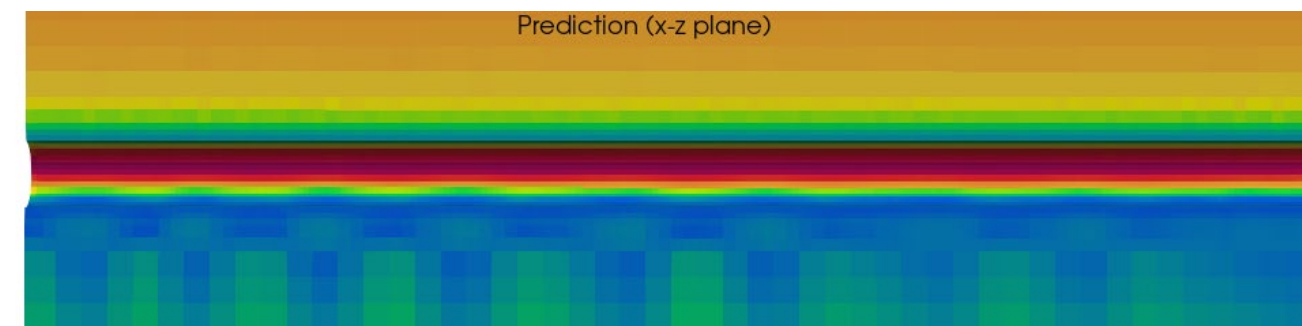
Air flow

(x-z)

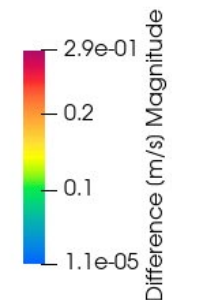
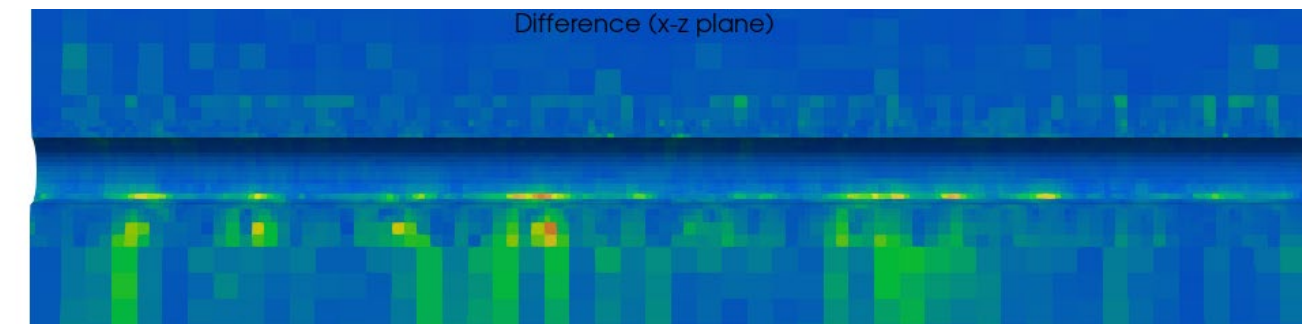
Original (x-z plane)



Prediction (x-z plane)



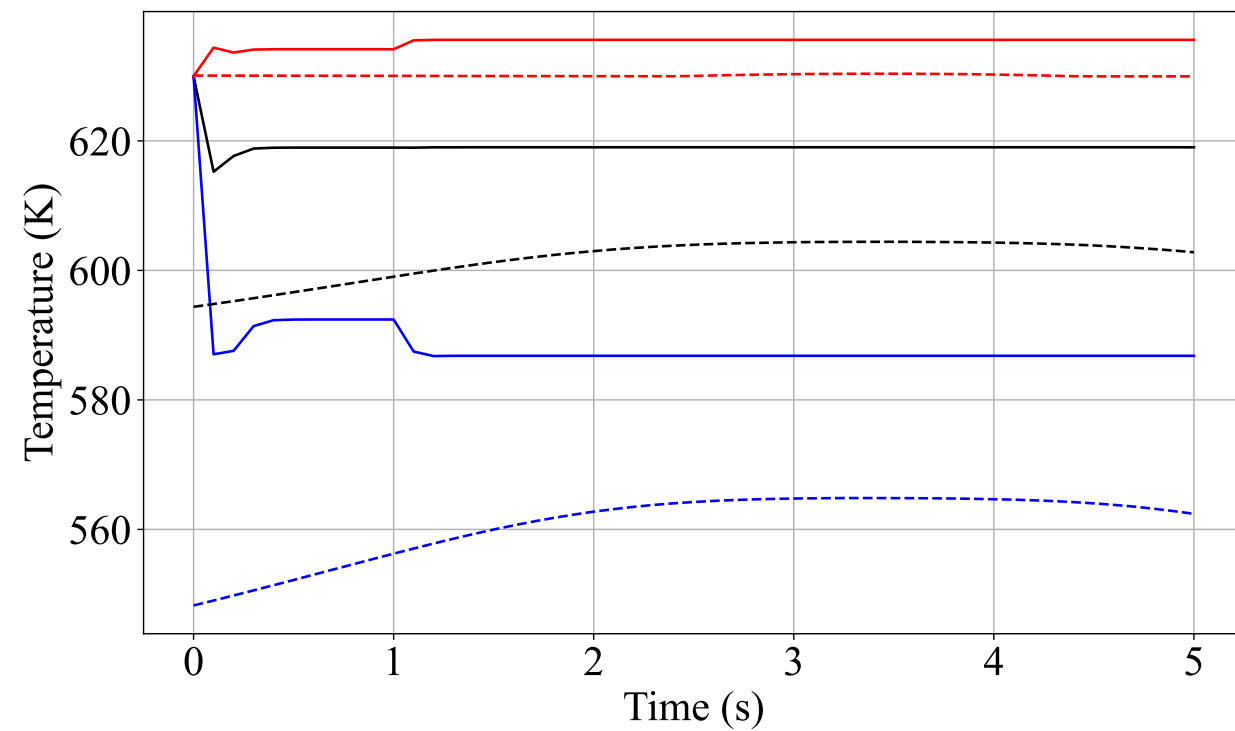
Difference (x-z plane)



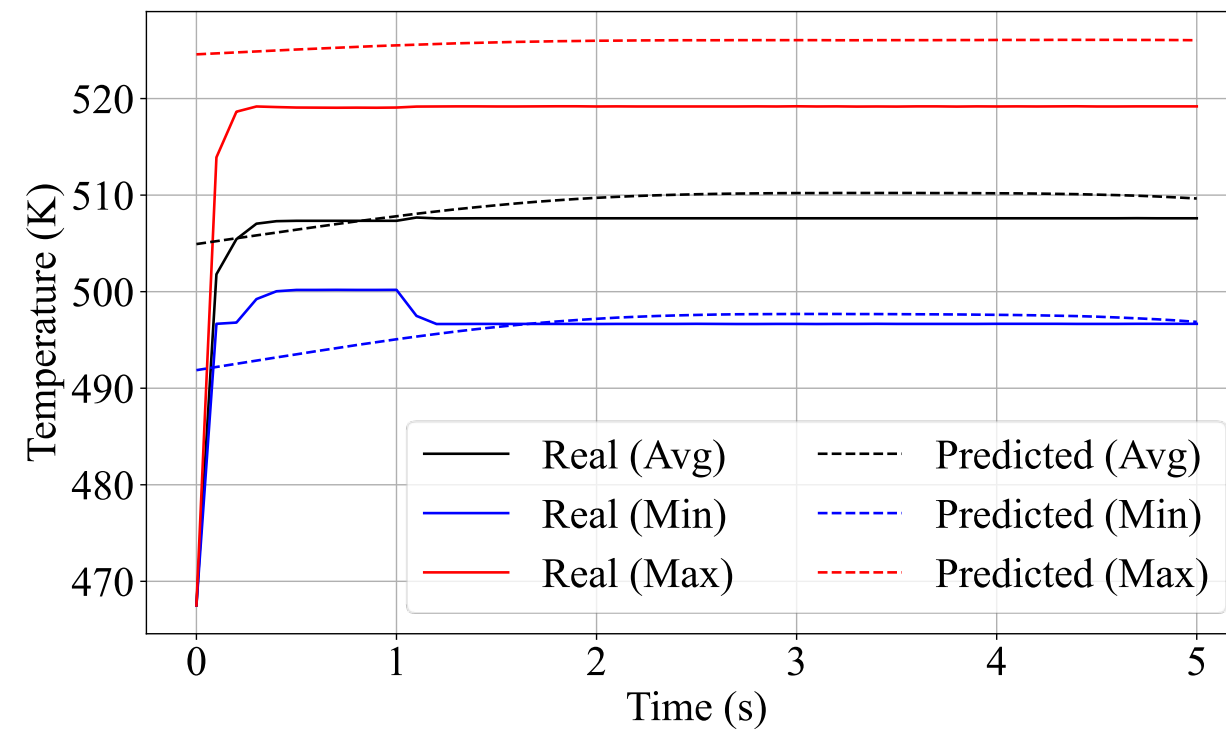
- For velocity, the prediction shows a good agreement with the original solution

# Temperature prediction over time for new design

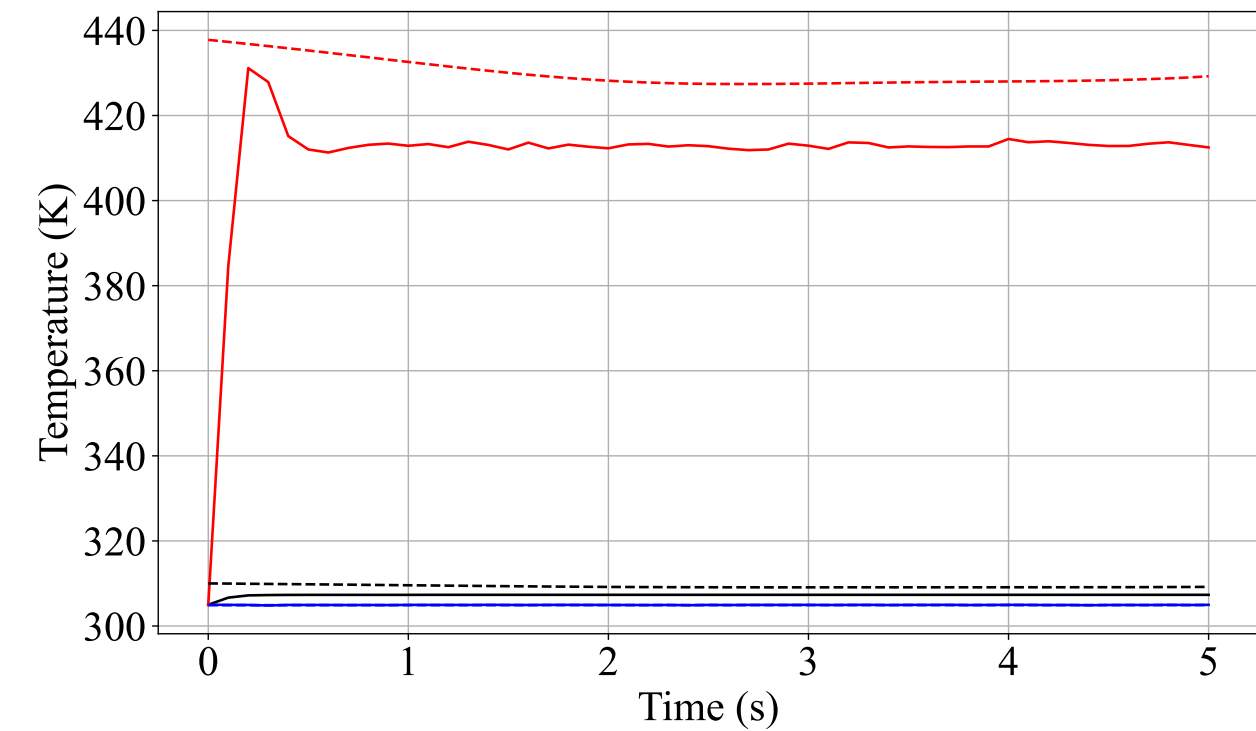
Gas flow



Solid pipe



Air flow



- The ROM matches closely the average (Avg), minimum (Min) and maximum (Max) temperature over time of the reactor

# Conclusions & Outlook



# Conclusions

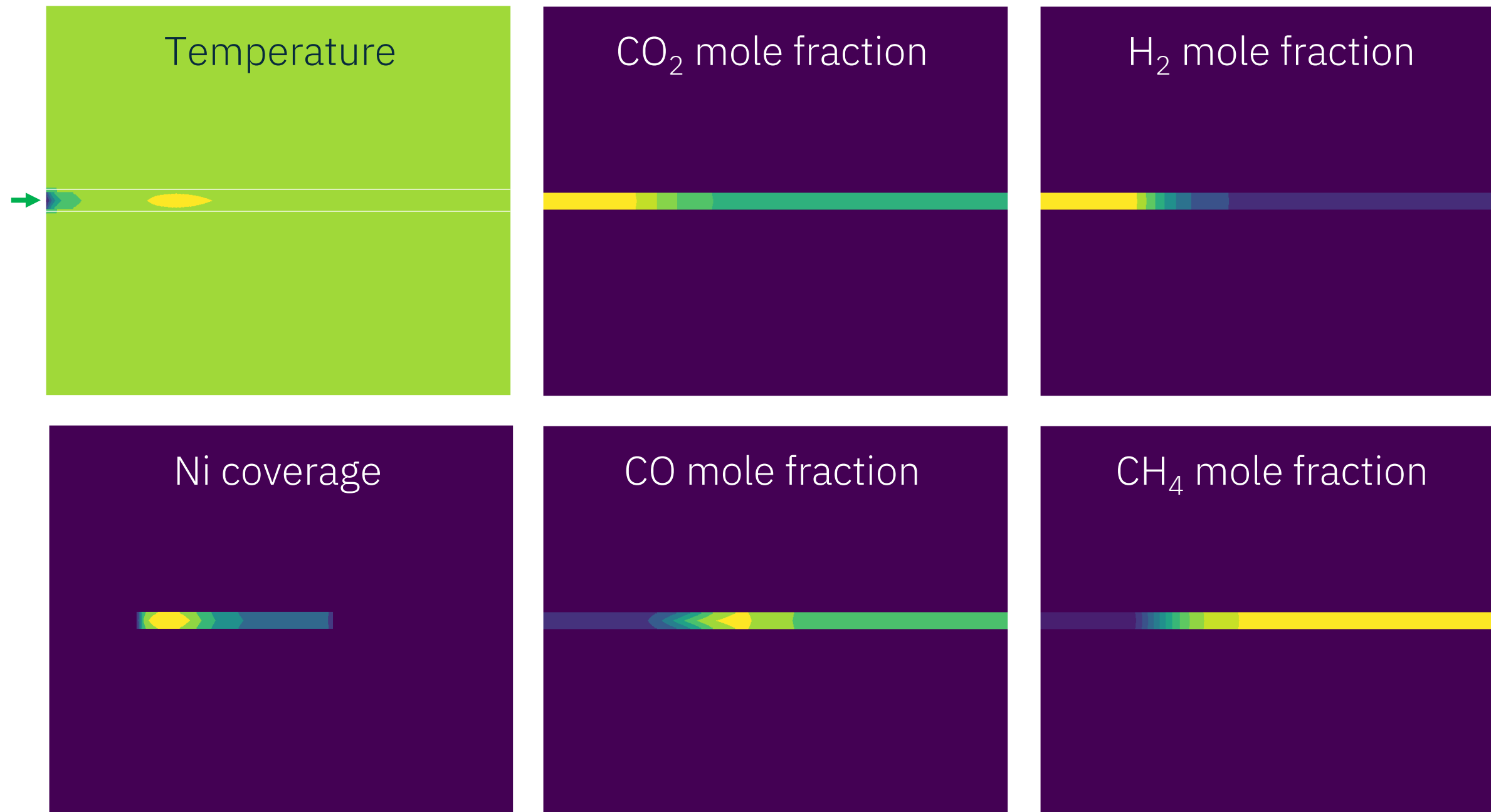
- We implemented a workflow in modeFRONTIER 2025R2 that enables to develop ROM of chemical reactors based on Converge CFD reactor simulations
- Overall computational costs and time:

DoE	ROM training	ROM prediction
<ul style="list-style-type: none"> <li>– Executed on HPC using 2 nodes @ 48 cores</li> <li>– Time: 30 hours</li> <li>– File size: 800 MB per design</li> </ul>	<ul style="list-style-type: none"> <li>– Executed on Laptop using 1 core</li> <li>– Time Gas Flow: 5m 40s</li> <li>– Time Solid Pipe: 5m 26s</li> <li>– Time Air Flow: 54m 27s</li> <li>– File size Gas Flow: 8.6 MB</li> <li>– File size Solid Pipe: 6.3 MB</li> <li>– File size Air Flow: 110.9 MB</li> </ul>	<ul style="list-style-type: none"> <li>– Executed on Laptop using 1 core</li> <li>– Time Gas Flow: 8m 51s for 51 time steps</li> <li>– Time Solid Pipe: 8m 41s for 51 time steps</li> <li>– Time Air Flow: 31m 35s for 51 time steps</li> </ul>

- ROM on a laptop 1-core takes ~32m vs. 3D-CFD on 48-core machine takes ~78.5m

# Outlook

- Extension of the current CFD model by including porous flow for the fixed bed and a detailed surface reaction mechanism



Converge CFD v3.1.9 reactor simulation

Reaction mechanism by Rakhi et al (2022)

Air temperature around the reactor pipe is at 623 K

$H_2/CO_2 = 2/1$

125 ml/min at STP

Ni/Al<sub>2</sub>O<sub>3</sub> spherical pellets (Ø=1mm)

# Acknowledgement

- Special Thanks to Saurabh Sharma and Arnim Brueger for supporting this development
- Special Thanks to the ESTECO team for providing the modeFRONTIER software licenses
- Thanks to CONVERGE for providing the CONVERGE CFD software licenses

This project is funded by the German government with funds from the Structural Development Act (Strukturstärkungsgesetz) for coal-mining regions and co-financed with funds from the state of Brandenburg.

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