Development of equipment design tools from experimental data using the example of autothermal reforming

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ThyssenKrupp Uhde

Agenda

- Introduction
  - Autothermal reformer (ATR)
  - ThyssenKrupp Uhde‘s pilot plant
- Experimental series
  - Soot formation boundary
  - Methane conversion
- Development of ATR design tools
  - One dimensional calculation
  - CFD calculation
  - Automated design optimization
- Conclusion and outlook

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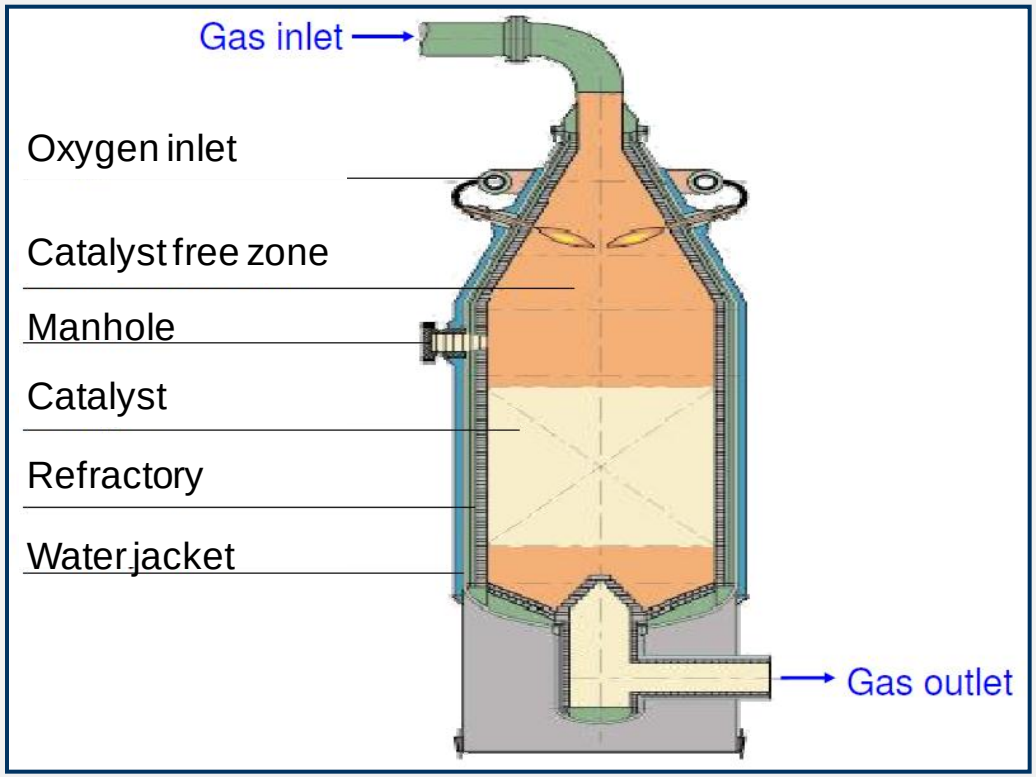
Introduction
Autothermal reformer



Alternative to primary and secondary reformer

Internal heat generation

Main reactions:

$CH_4+2O_2 \rightarrow CO_2+2H_2O$

$2CH_4+O_2 \rightarrow 2CO+4H_2$

→ Autotherm

Catalyst free reforming

$CH_4+H_2O \leftrightarrows CO+3H_2$

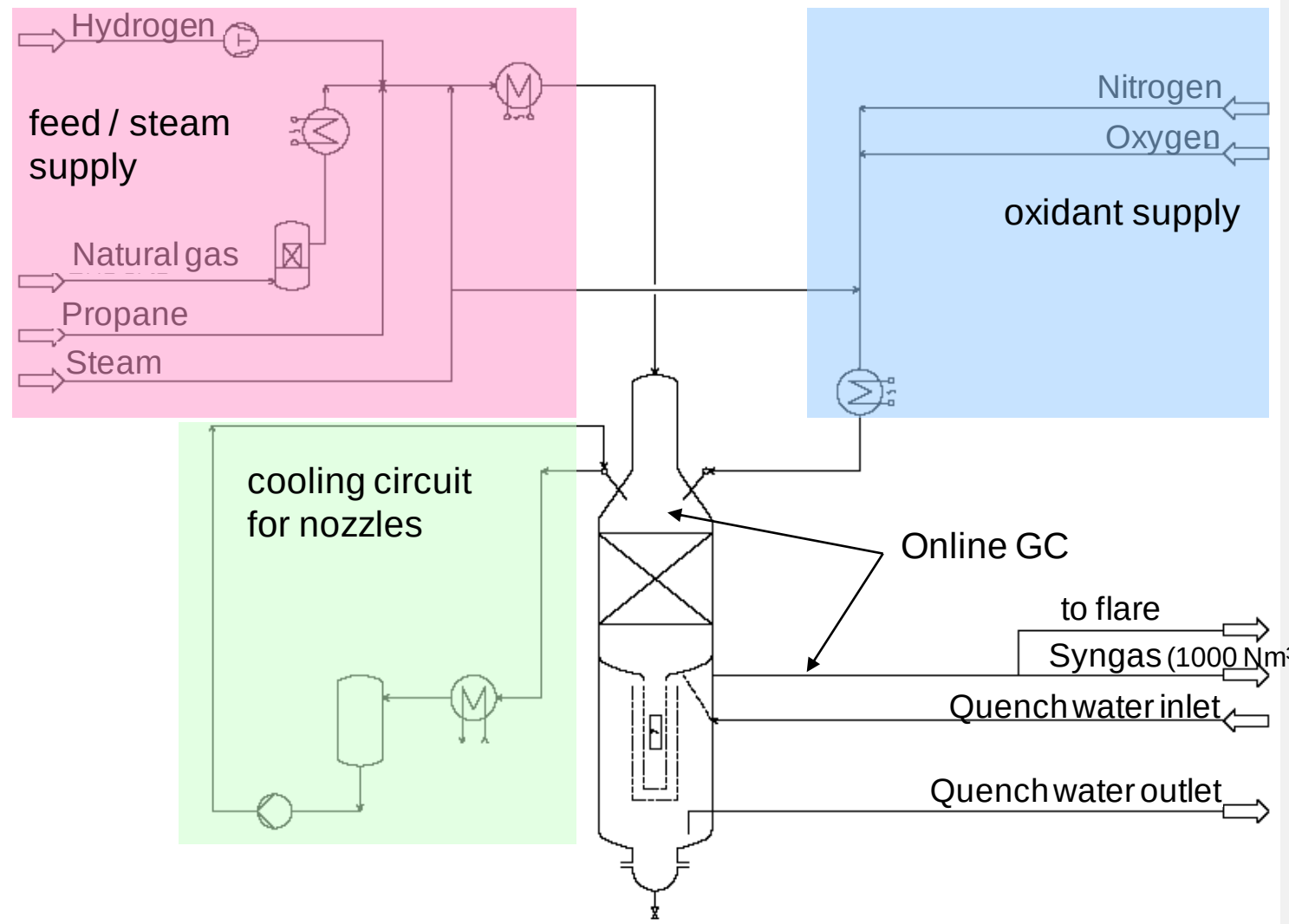
$CO+H_2O \leftrightarrows CO_2+H_2$

Catalytic reaction

→ Small T-Approach

Introduction

ThyssenKrupp Uhde's pilot plant



Introduction
ThyssenKrupp Uhde's pilot plant

- Starting in 2009

- Two online analysis points (GC)
  - H_2 - CO - CO_2
  - N_2 - CH_4 - O_2/Ar

- About 2000 experiments differing in
  - Pressure
  - Temperature
  - Steam to carbon ratio
  - Nitrogen content
  - Amount of catalyst
  - Reactor load
  - Geometry

Togliatti, Russia

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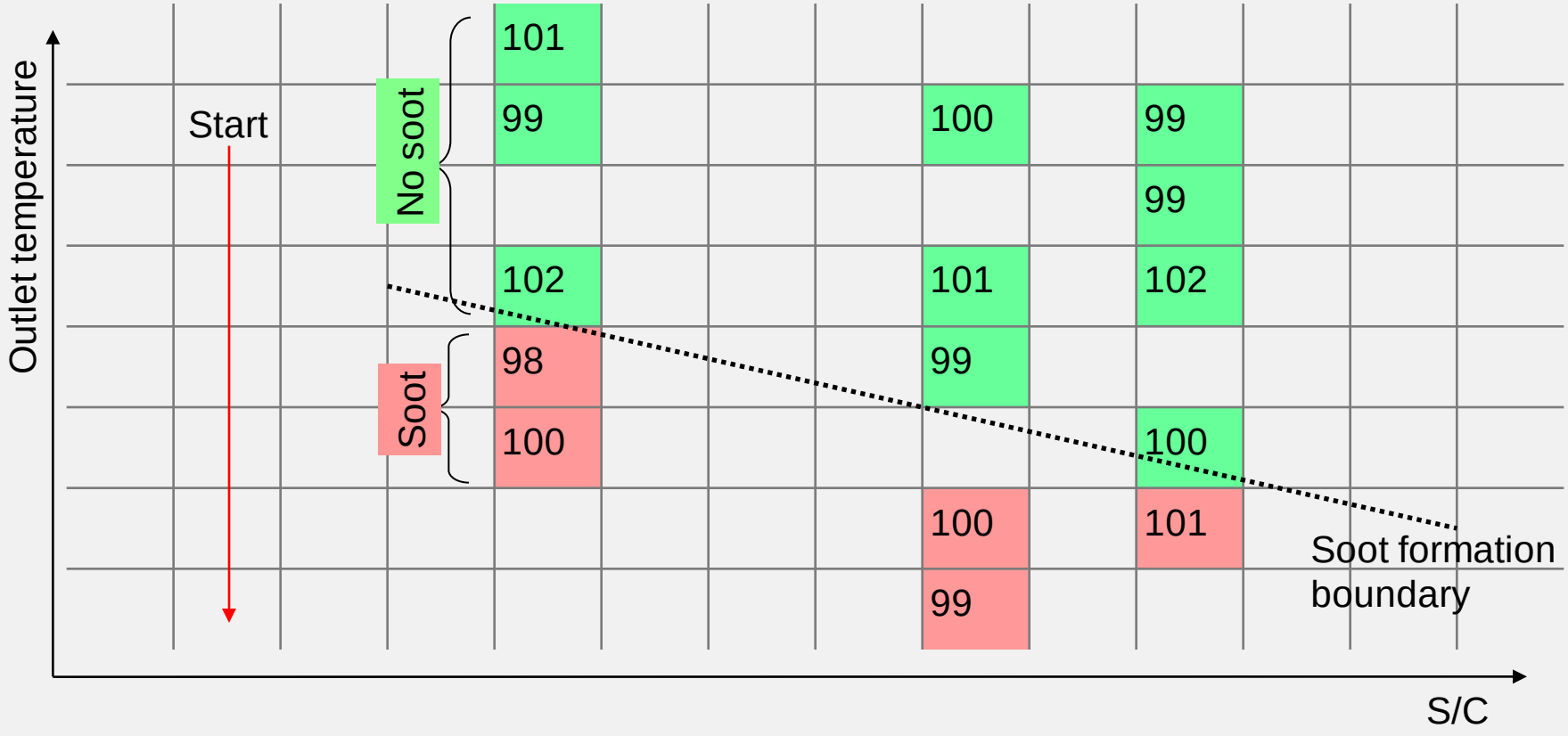
Experimental series

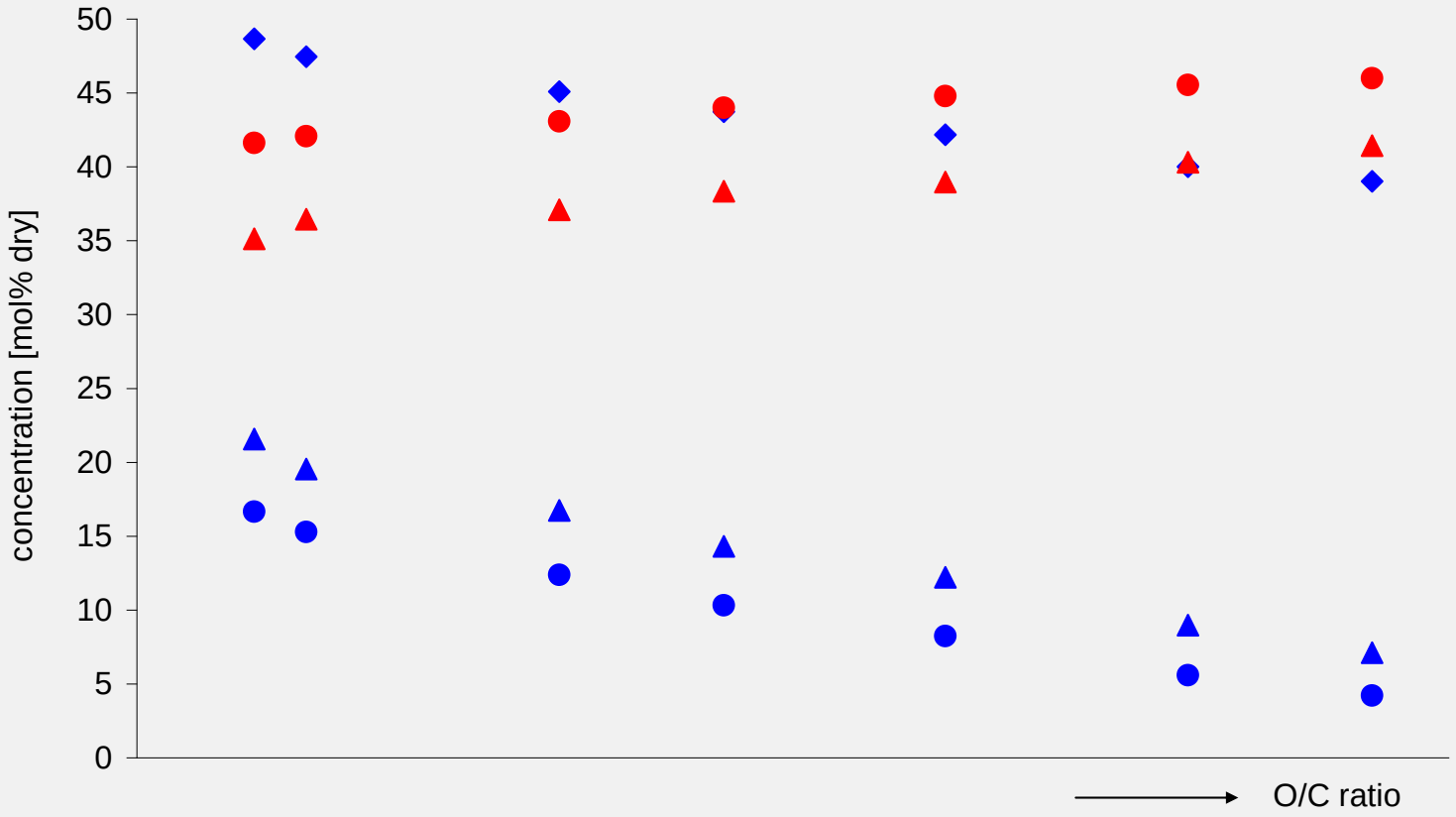
Soot formation boundary



Constant pressure, constant N_2 content, constant load (98%-102%)
Experiments without catalyst

Experimental series

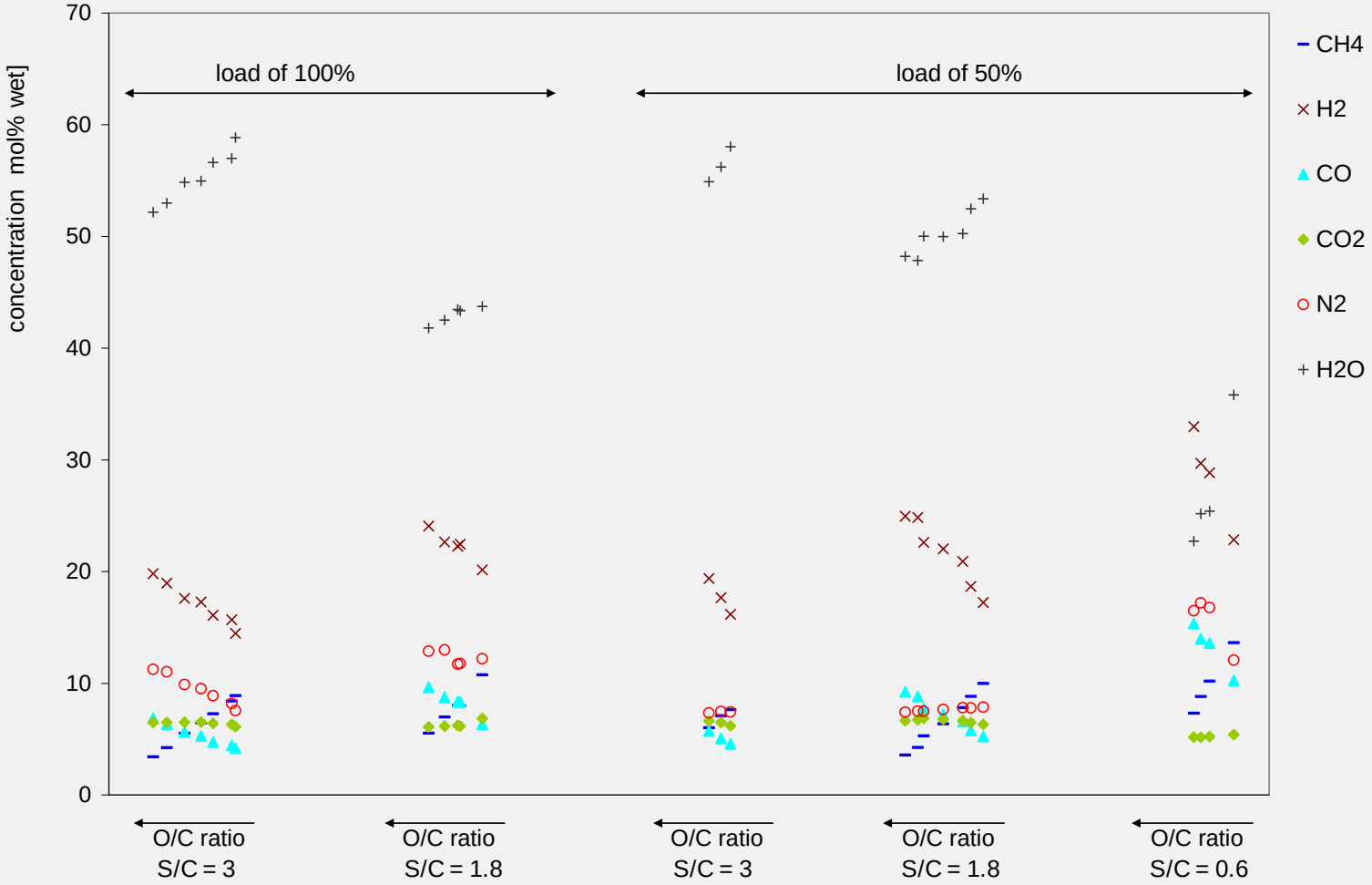
Methane conversion



Concentration of H_2 (red) and CH_4 (blue) at inlet condition (◆), upstream catalyst bed (▲) and downstream the catalyst bed (●)

Experimental series

Methane conversion



Concentration upstream catalyst bed, constant pressure, constant nitrogen content

ThyssenKrupp Uhde

ThyssenKrupp

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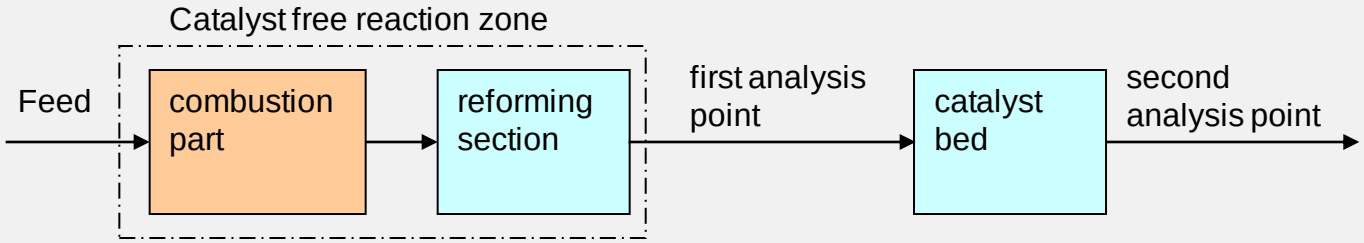
Development of ATR design tools

One dimensional - model



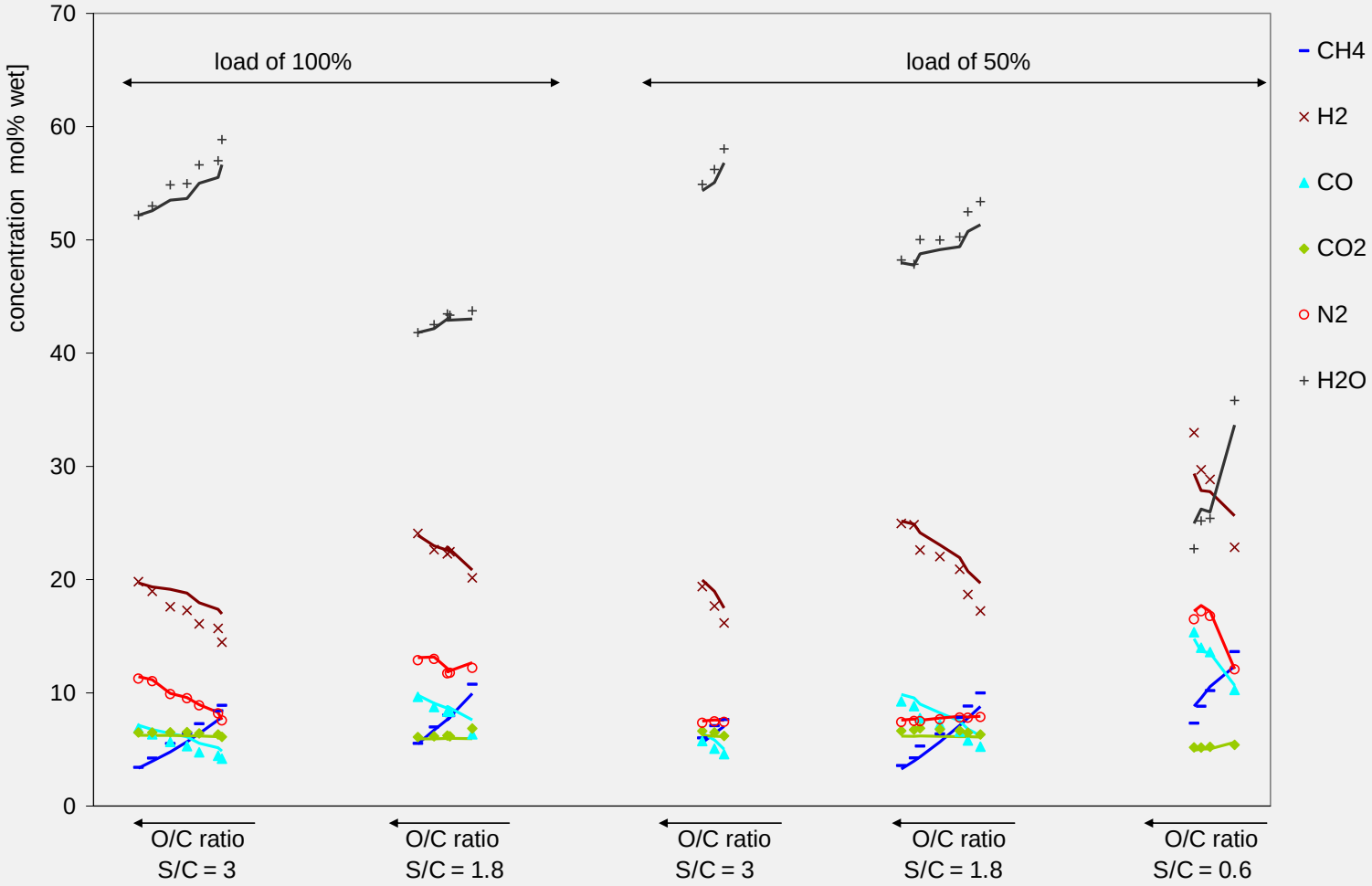
C_nH_{2n+2}	+	n 0.5 O_2	→	n CO	+	2n H_2
CO	+	0.5 O_2	→	CO_2		
H_2	+	0.5 O_2	→	H_2O		
CH_4	+	H_2O	→	CO	+	3 H_2
CO	+	H_2O	→	CO_2	+	H_2

Kinetic approach for reforming:

$$r = A \cdot \exp\left(-\frac{E_A}{RT}\right) \cdot p_{CH_4}^{\alpha} \cdot p_{H_2O}^{\beta} \cdot p_{CO}^{\gamma} \cdot p_{H_2}^{\delta}$$

Development of ATR design tools

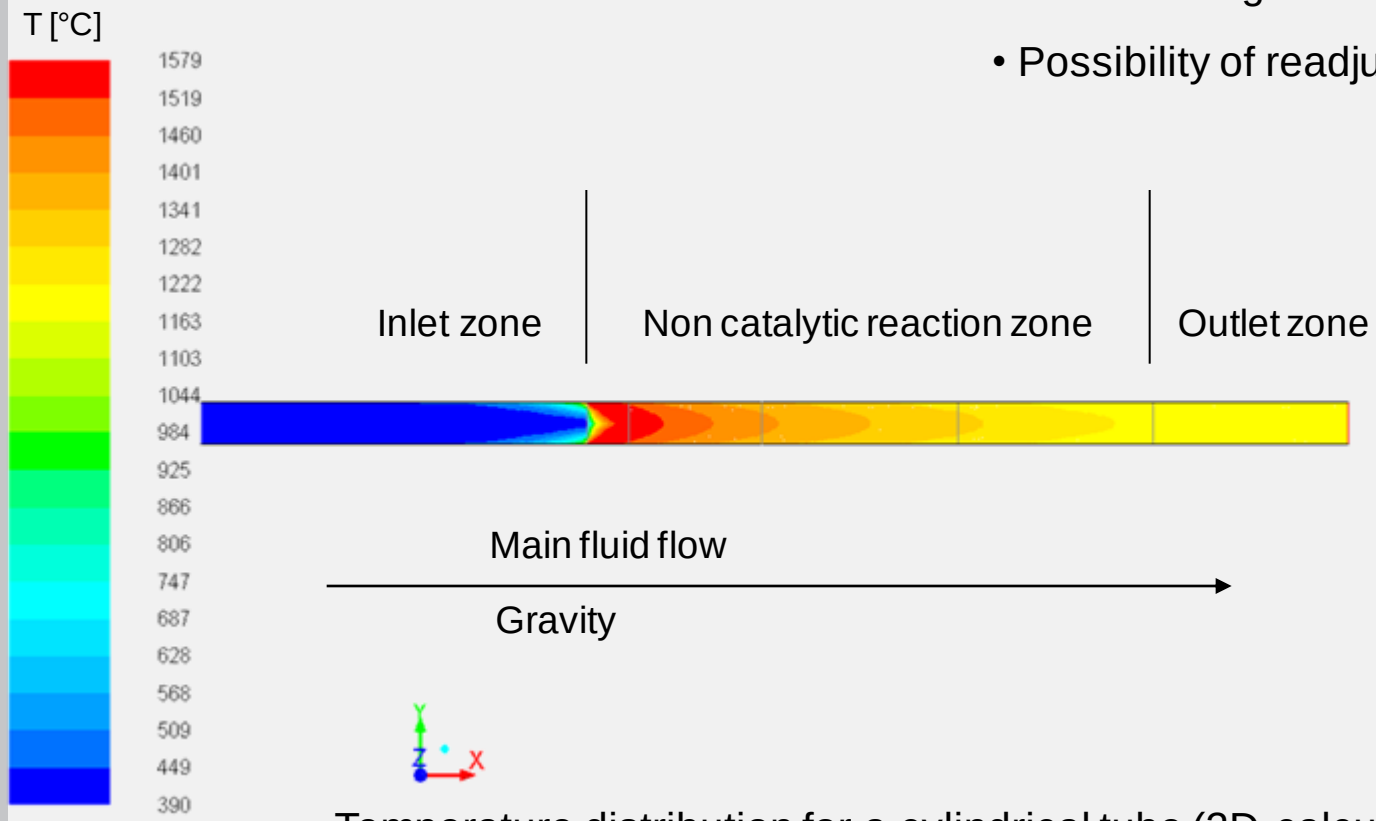
One dimensional – conversion results



Concentration upstream catalyst bed, constant pressure, constant nitrogen content

Development of ATR design tools
CFD calculation – 2D

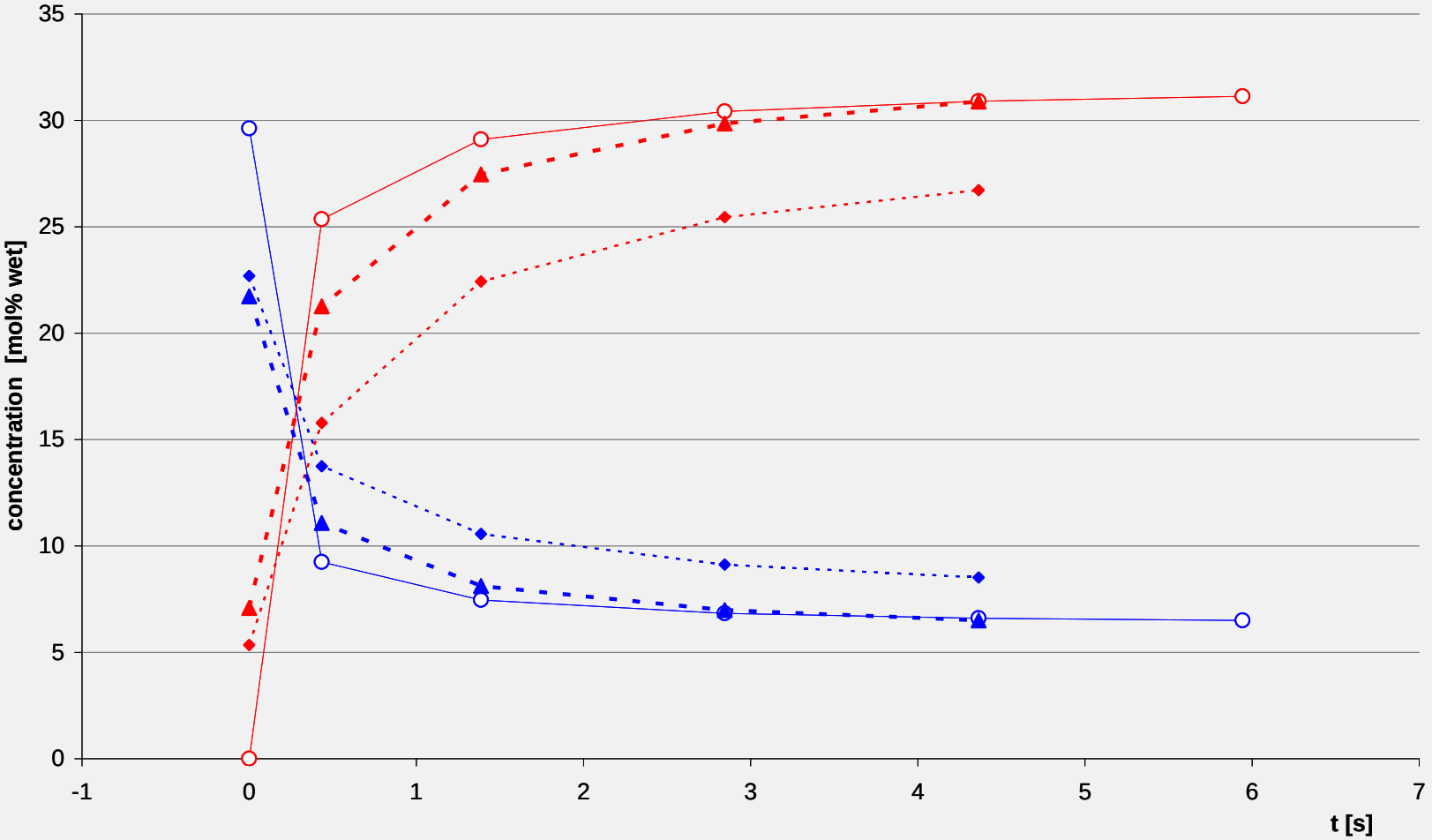
- 2D-Model for fast simulation
- For checking the transfer of kinetics
- Possibility of readjusting parameters



Temperature distribution for a cylindrical tube (2D-calculation)

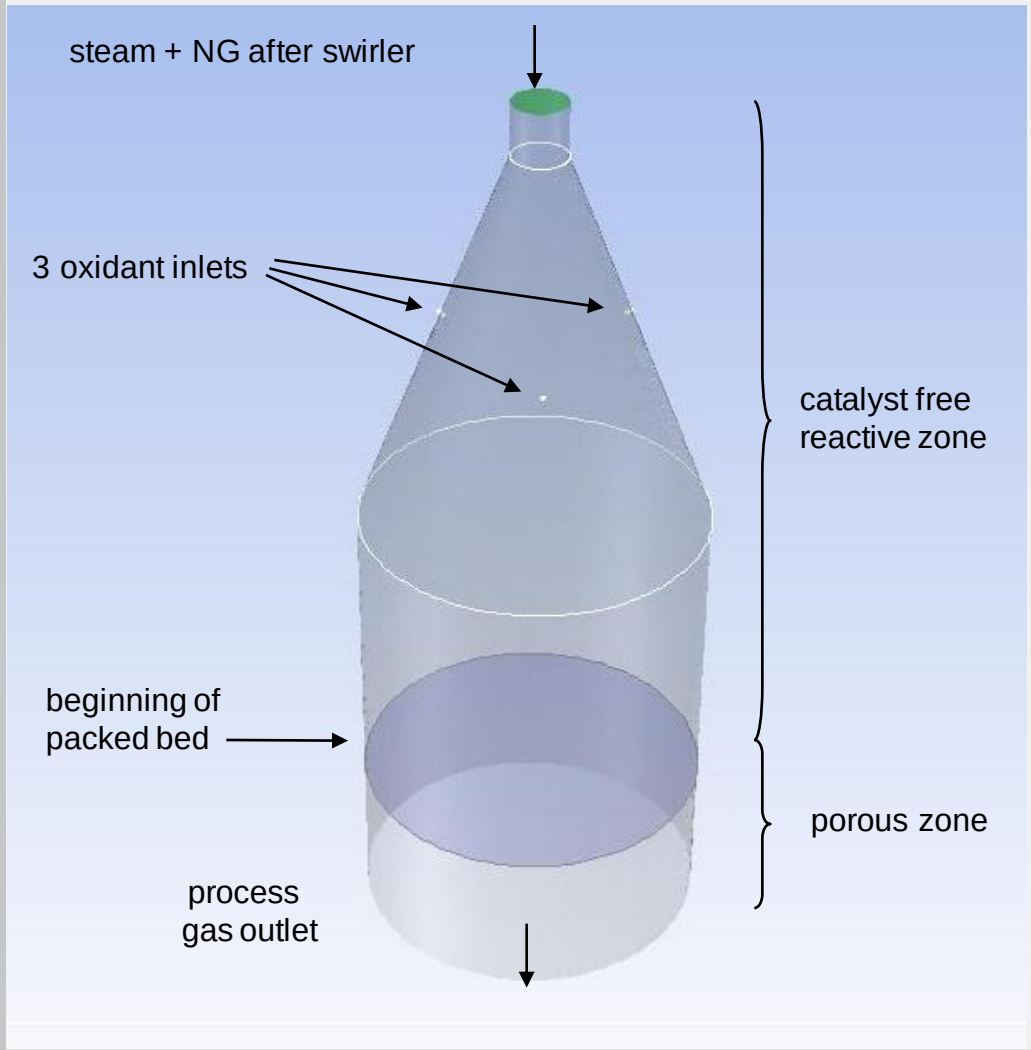
Development of ATR design tools

CFD calculation – 2D



Concentration of H_2 (red) and CH_4 (blue) simulated with AspenPlus (solid) and Fluent (dashed)

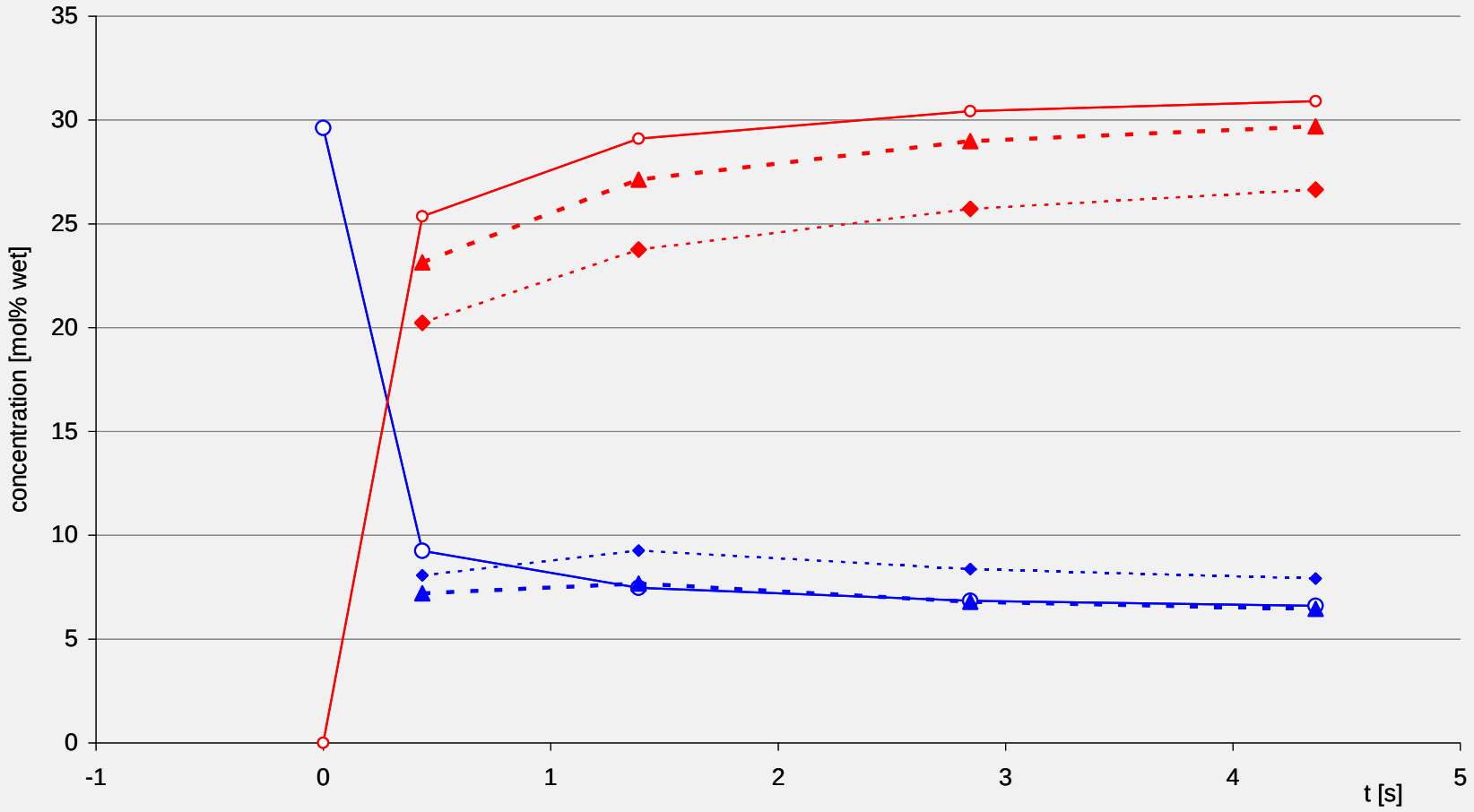
Development of ATR design tools
CFD calculation – 3D



- Geometry like ATR pilot plant
- Swirled feed/steam mixtures
- Narrow meshing around oxidant nozzles
- Porous zone without reaction

Development of ATR design tools

CFD calculation – 3D



Concentration of H_2 (red) and CH_4 (blue) simulated with AspenPlus (solid) and Fluent (dashed)

Development of ATR design tools

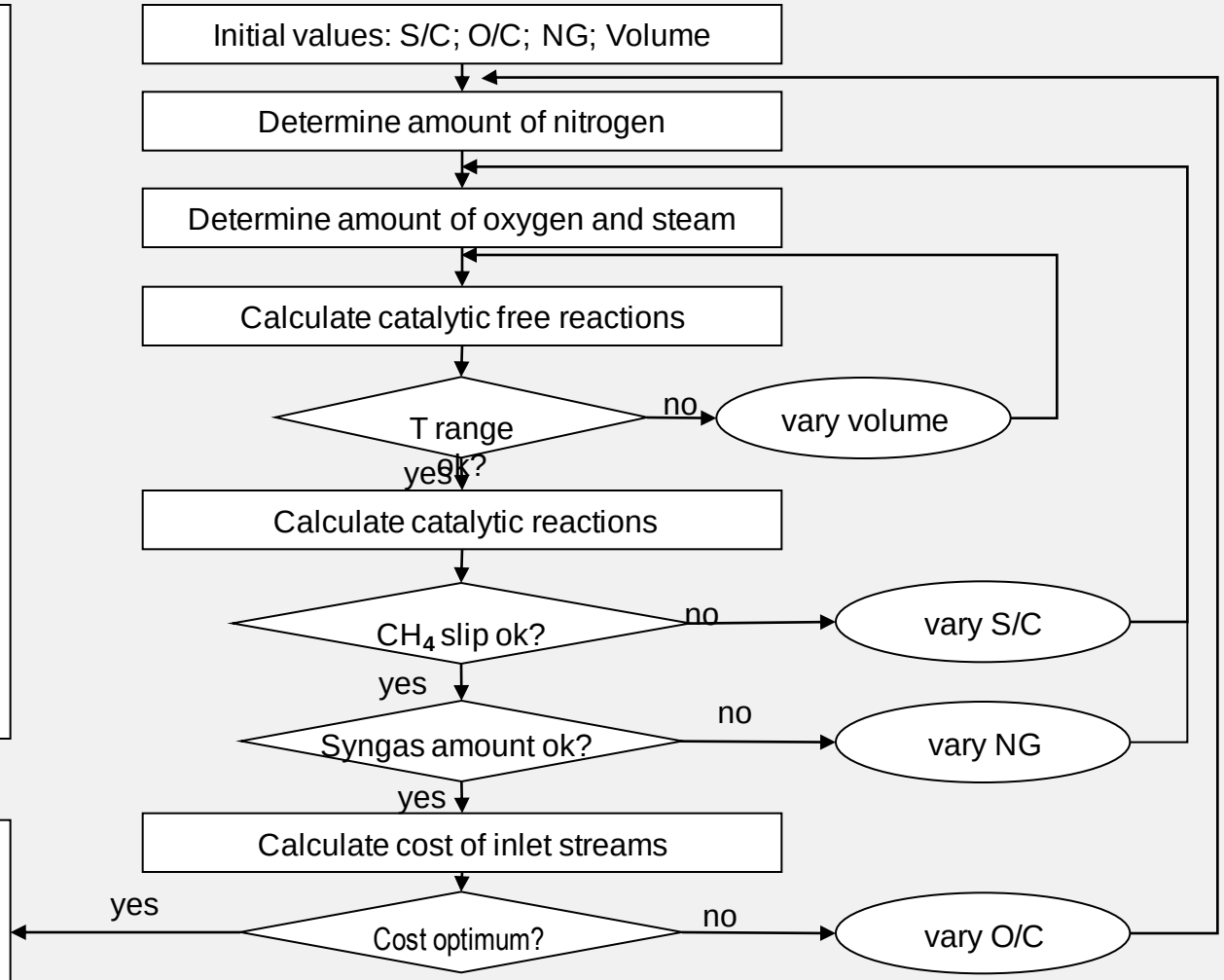
Automated design optimization (1D)

User Input

Specifications:
- Feed temperature
- Feed composition
- Pressure
- Specific costs

Requirements:
- H_2 : N_2 - ratio
- T-range
- CH_4-slip
- Amount of syngas

Results:
- Feed streams
- Volumes



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Conclusion and outlook

Current status:

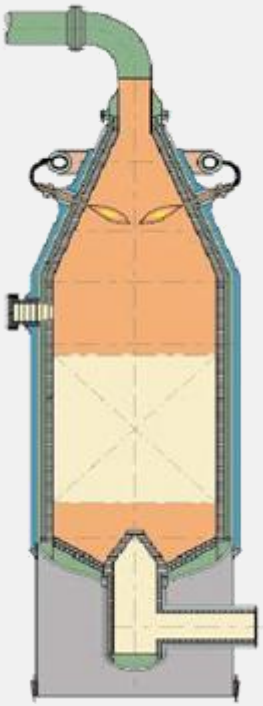
- Analysis of more than 2000 experimental data points
- Development of kinetics for catalyst free zone
- Development of three-dimensional CFD-Model

Next steps:

- Completion of automated optimization program
- Extension of Fluent model

→ **Quickly identify the most efficient ATR-based process for any given plant requirement**

Thank you very much



for your attention!

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