Consumet - Model reduction software, its approach, and its rationale

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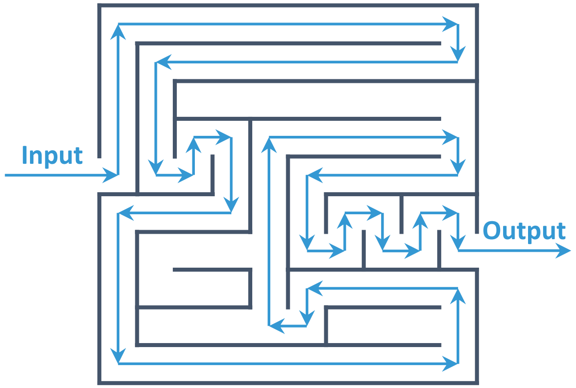
Outline

- What is a reduced order model and why are they important?
- How are reduced order models calculated?
- What is included in Consumet?
    - Constraints for sampling domain reduction
    - Example: water-gas shift section of H_2 production
- How was Consumet used within ELEGANCY?
- Conclusion

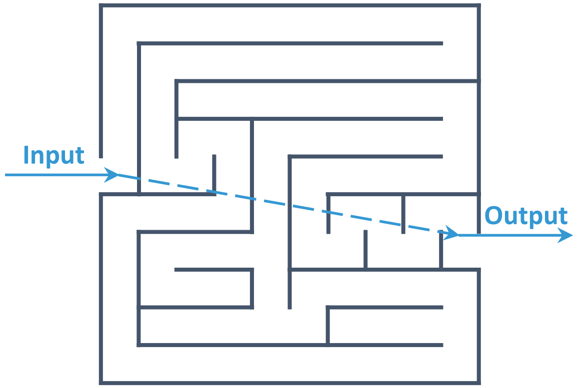
What is a reduced-order model and why are they important?



Detailed model

- Computational demanding (first principle) models

➢ **<u>Cannot</u>** be used in high level models (complexity/coupling)



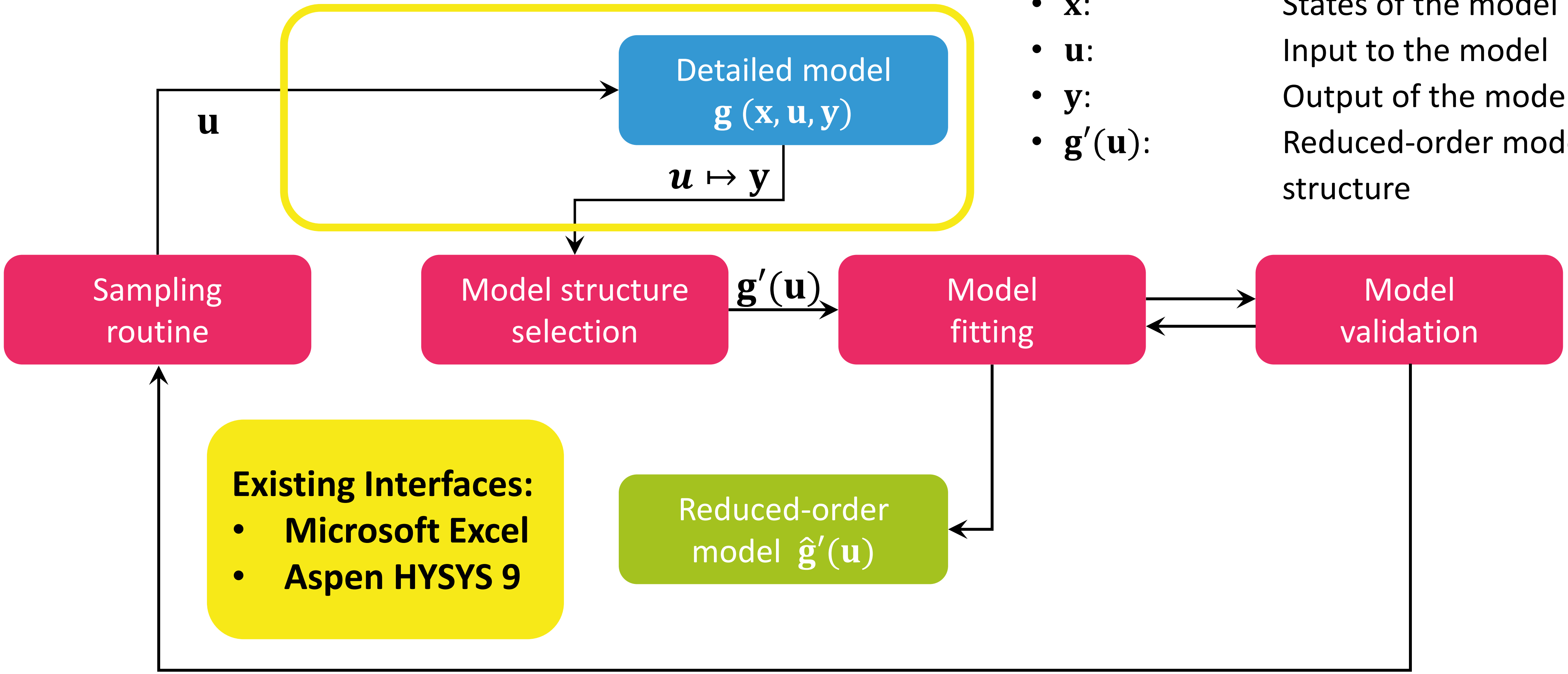
Reduced-order model

- Reduced-order model of computational demanding (first principle) models

➢ **<u>Can</u>** be used in high level models (fast to solve, easy to implement)

How are reduced order models calculated?

- $\mathbf{x}$: States of the model
- $\mathbf{u}$: Input to the model
- $\mathbf{y}$: Output of the model
- $\mathbf{g}'(\mathbf{u})$: Reduced-order model structure



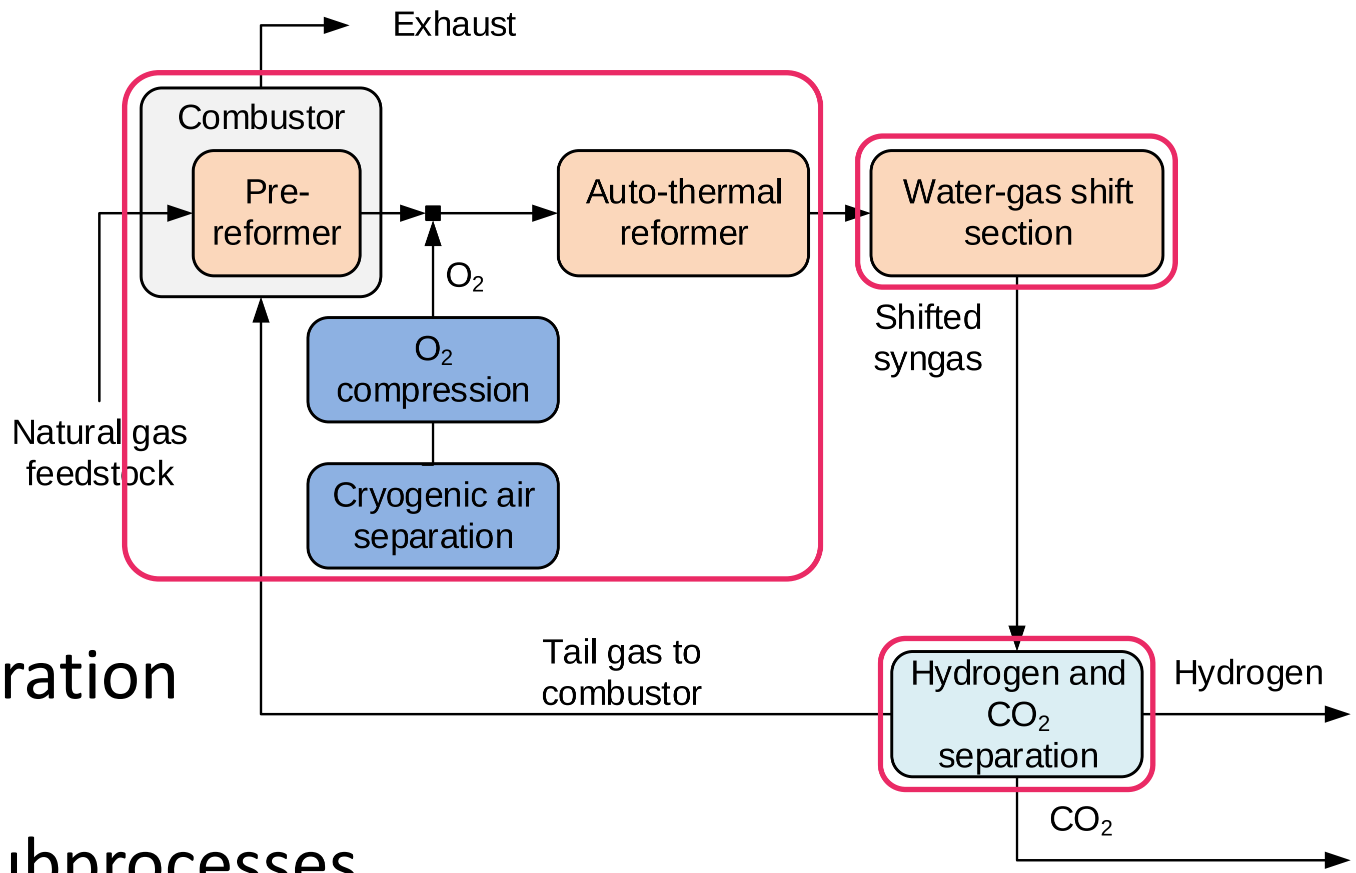
What is included in Consumet?

- Developed in Python using Pyomo and free solver
- Calculation of reduced-order models either *via* sampled data or interlink with detailed model
- Allows for:
  - Static (Batch) sampling
  - Adaptive sampling based on **error maximization sampling**
- Regression via **LASSO** and several information criteria
- Basis functions:
  - Taylor polynomials
  - Legendre polynomials
  - Chebyshev polynomials
  - Fourier series

What is now new (or special) in Consumet?

H_2 production with CCS

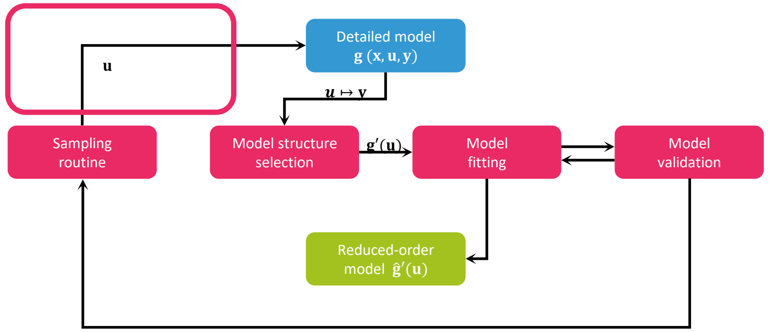
- Many process configurations:
  - Type of reforming reactor
  - Number of WGS reactors
  - What separation technologies



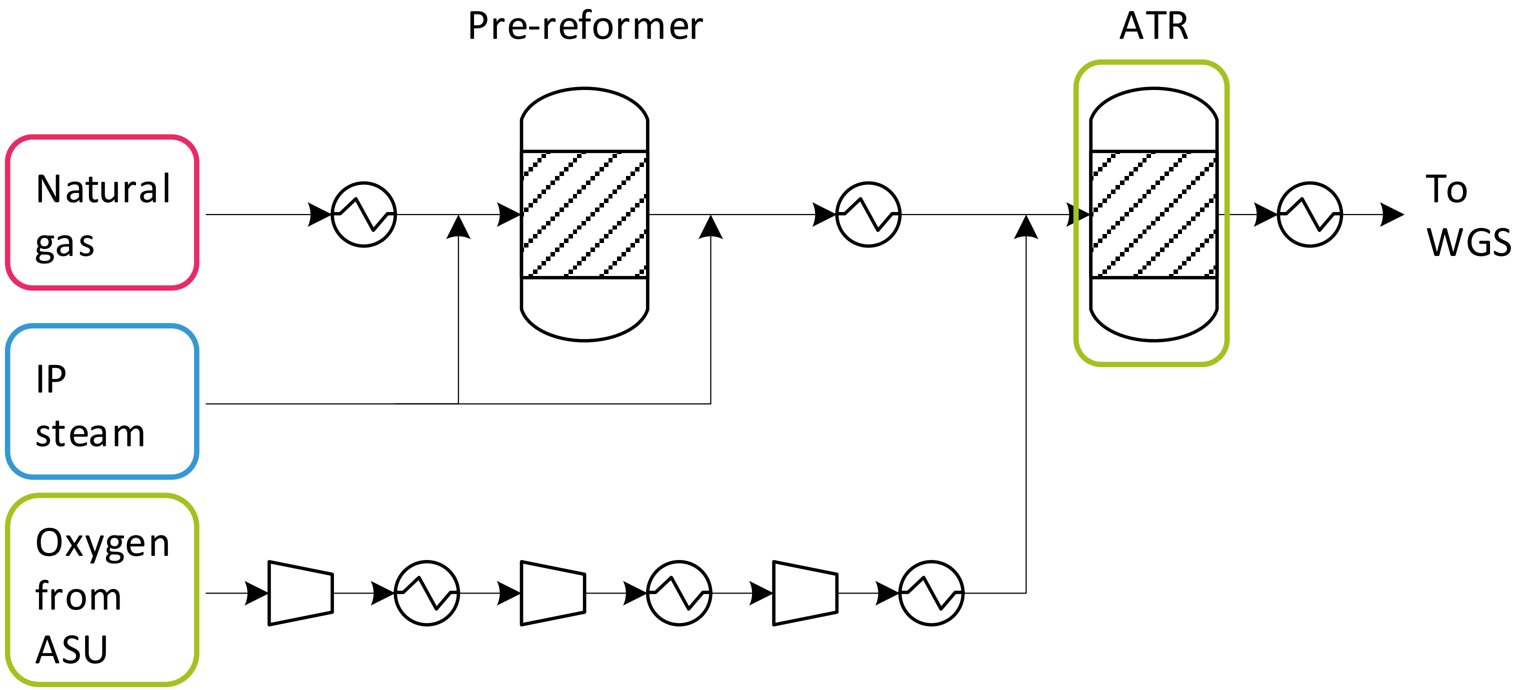
→ Hard to optimize case-dependent process configuration

→ Reduced order models of subprocesses for **superstructure optimization**

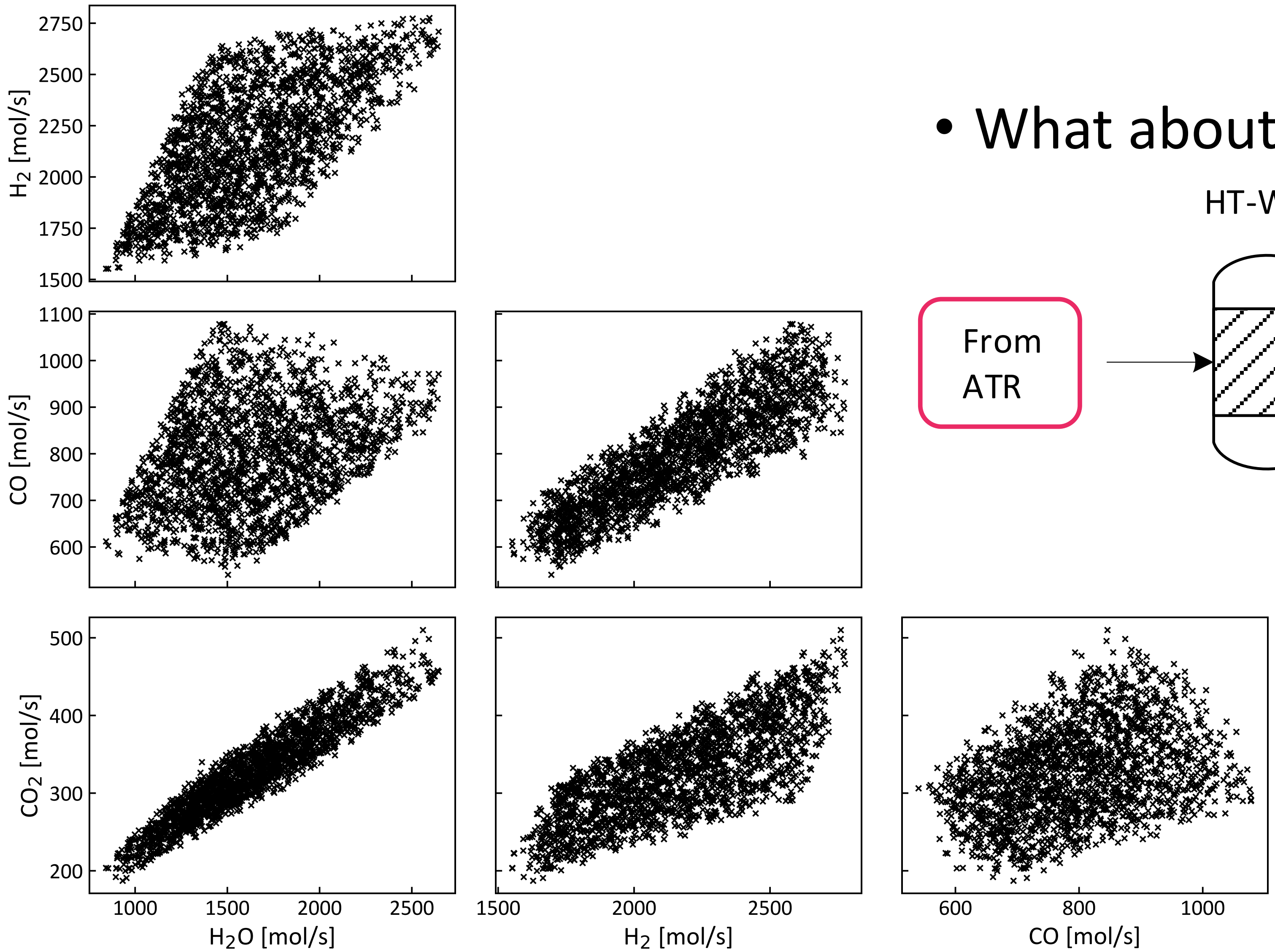
Constraints for independent variables



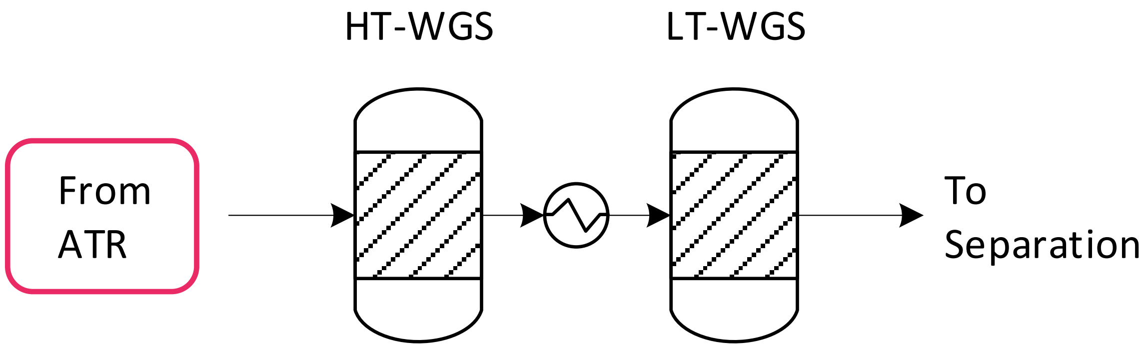
- Standard approach:
  - Sampling with box-constraints for the input variables
  - Potential introduction of ratios as new input variables
  - Potential introduction of "control structures"



Constraints for sampling domain reduction



- What about dependent sections?



- Box and ratio constraints result in large, un-necessary sampling
- Potential problems with model fitting

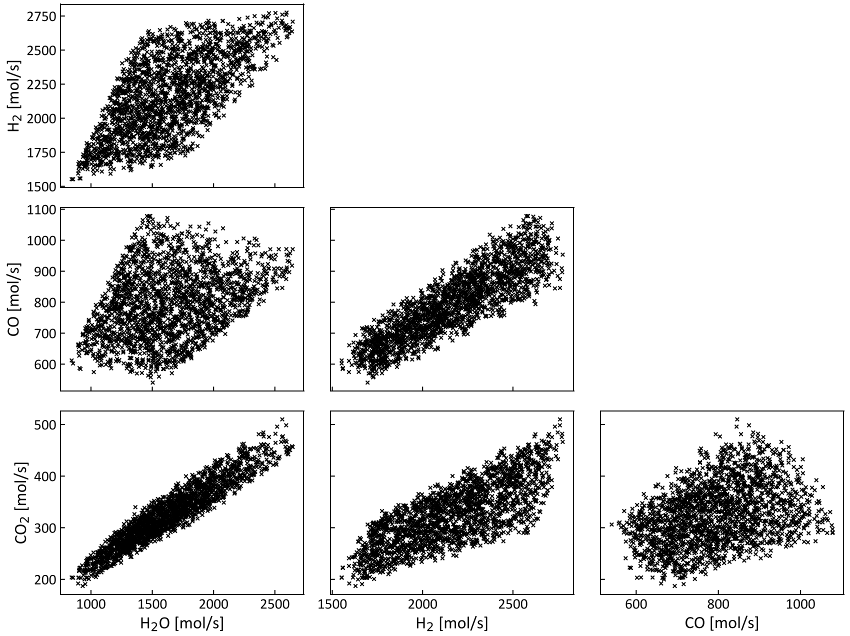
New constraints for sampling domain reduction

- Data-driven constraints:

$$\min\left(\dot{n}_i^{dat}\right) \le \dot{n}_i \le \max\left(\dot{n}_i^{dat}\right)$$

$$\dot{n}_j \min\left(\frac{\dot{n}_i^{dat}}{\dot{n}_j^{dat}}\right) \le \dot{n}_i \le \dot{n}_j \max\left(\frac{\dot{n}_i^{dat}}{\dot{n}_j^{dat}}\right)$$

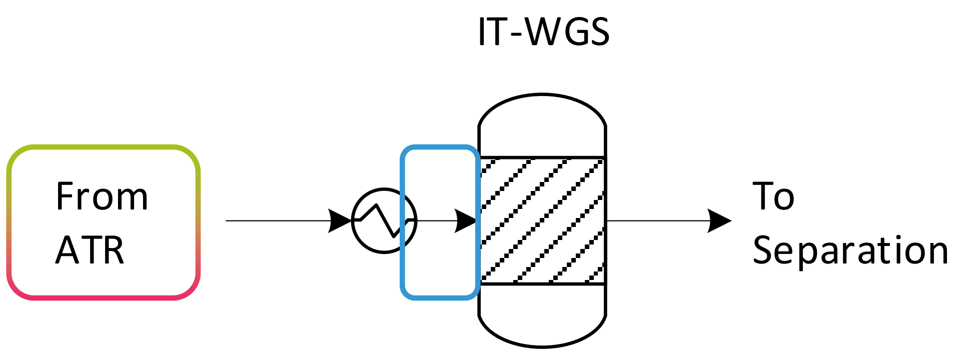
$$\min\left(\dot{n}_i^{dat} + \dot{n}_j^{dat}\right) \le \dot{n}_i + \dot{n}_j \le \max\left(\dot{n}_i^{dat} + \dot{n}_j^{dat}\right)$$



- Properties:
  - Convex set
  - Includes all points
  - Can also include some extra slack
  - Calculated from previous subprocesses

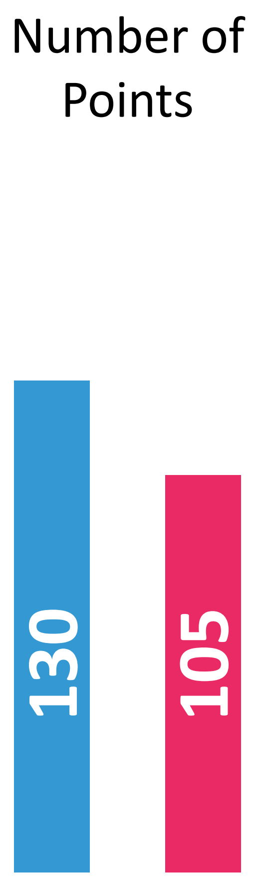
One water-gas shift reactor - description

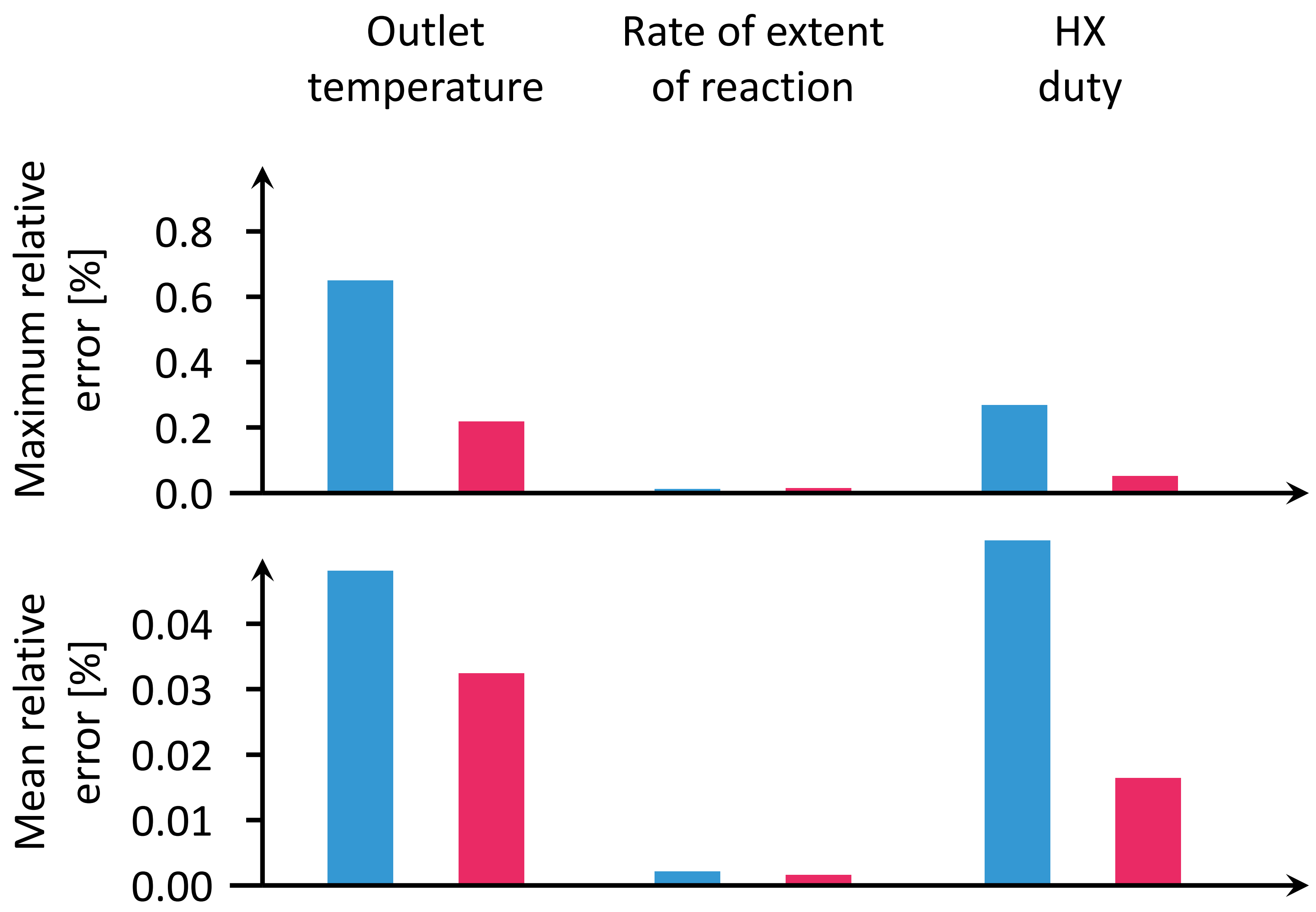
- Input variables:
  - inlet temperature cooler
  - inlet molar flowrates (CO, CO_2, H_2, and H_2O)
  - inlet temperature IT-WGS
- Output variables:
  - outlet temperature IT-WGS
  - rate of extent of reaction WGS
  - Duty cooler



- 2 000 points for calculating the constraints
- Basis function:
  - Third order Legendre polynomials
- 2 000 points for validation

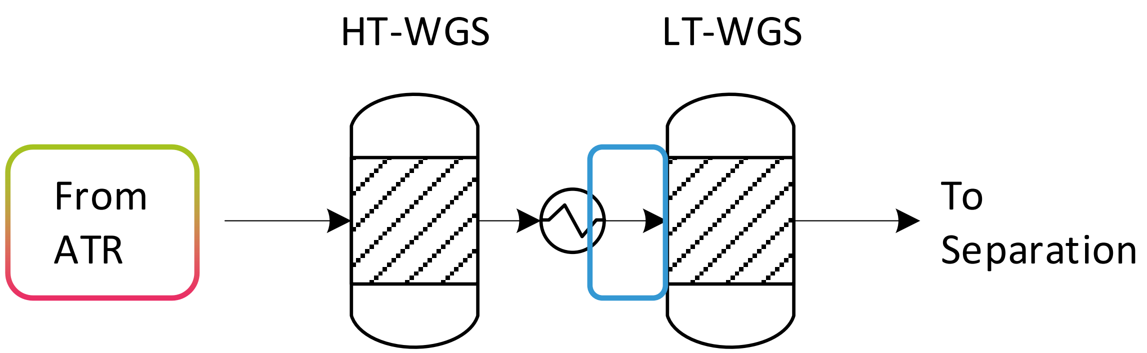
One water-gas shift reactor - results





Two water-gas shift reactor - description

- Input variables:
  - inlet temperature HT-WGS
  - inlet molar flowrates (CO, CO_2, H_2, and H_2O)
  - inlet temperature LT-WGS
- Output variables:
  - outlet temperature HT-WGS and LT-WGS
  - rate of extent of reaction WGS combined
  - duty cooler



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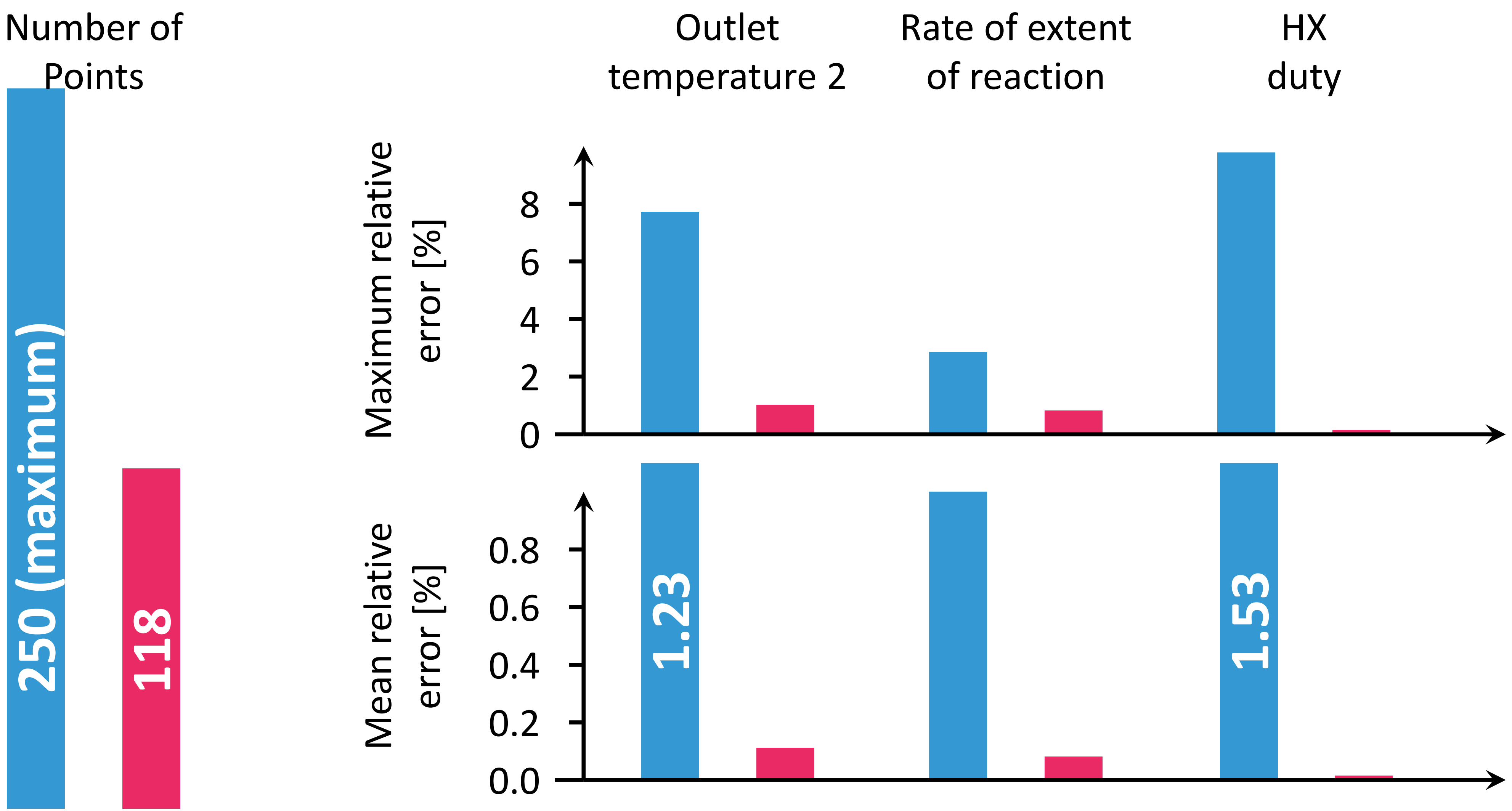
Two water-gas shift reactors - results



How was Consumet used within ELEGANCY?

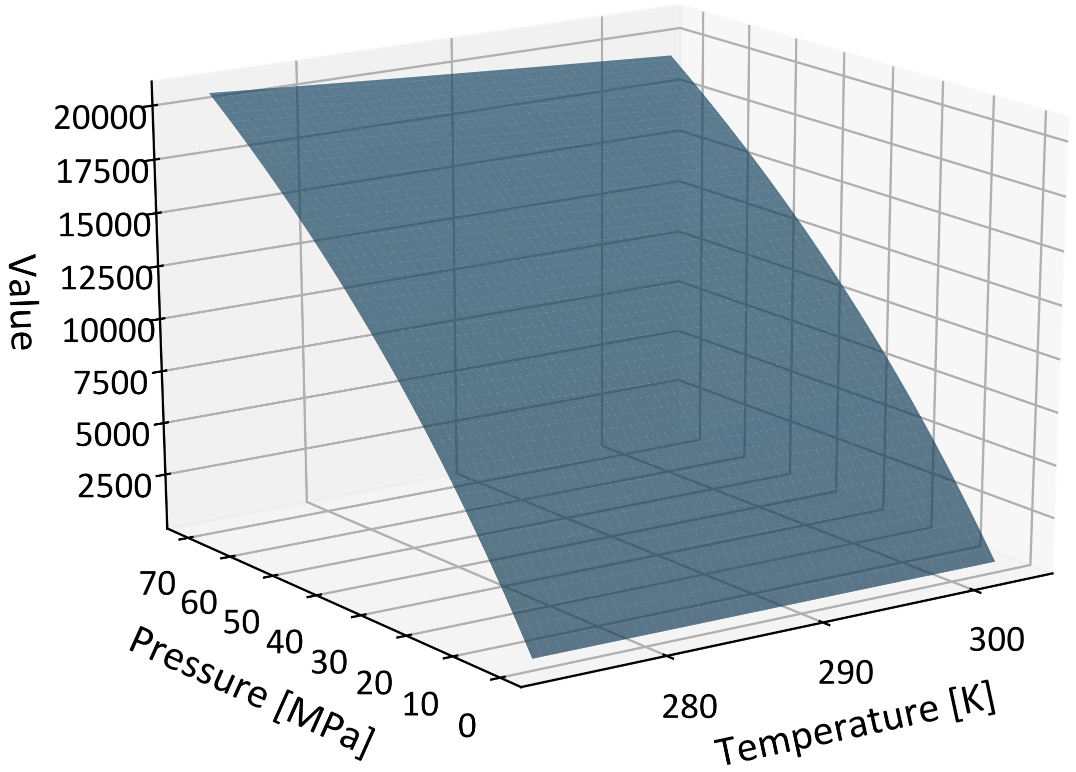
- Thermodynamic properties required in operational (dynamic) model for correct calculation of e.g. line packing of hydrogen
- Thermodynamic equations based on Helmholtz equation further developed in WP2 in software package TREND (Fortran)
- Problems:
  - Calculations computational expensive for large number of evaluations, typical in dynamic simulations
  - Coupling of TREND with Modelica not straight forward for fluid properties

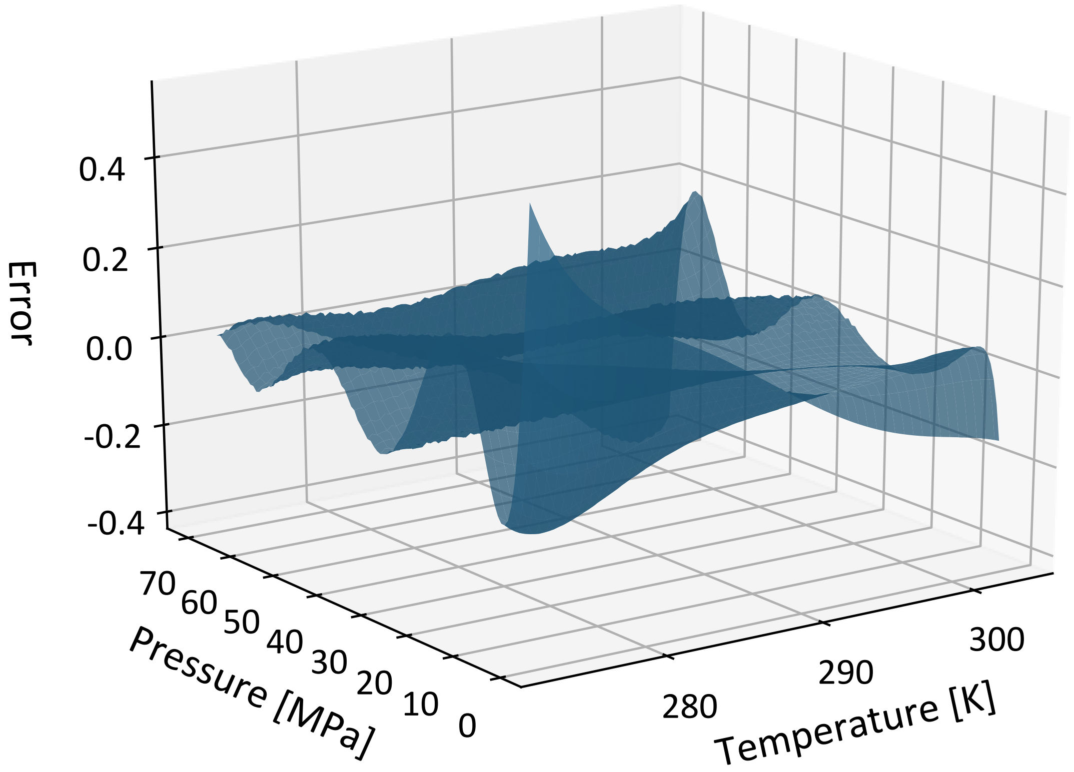
➢ Reduced order models calculated from TREND for application in operational model

Thermodynamic property ROM

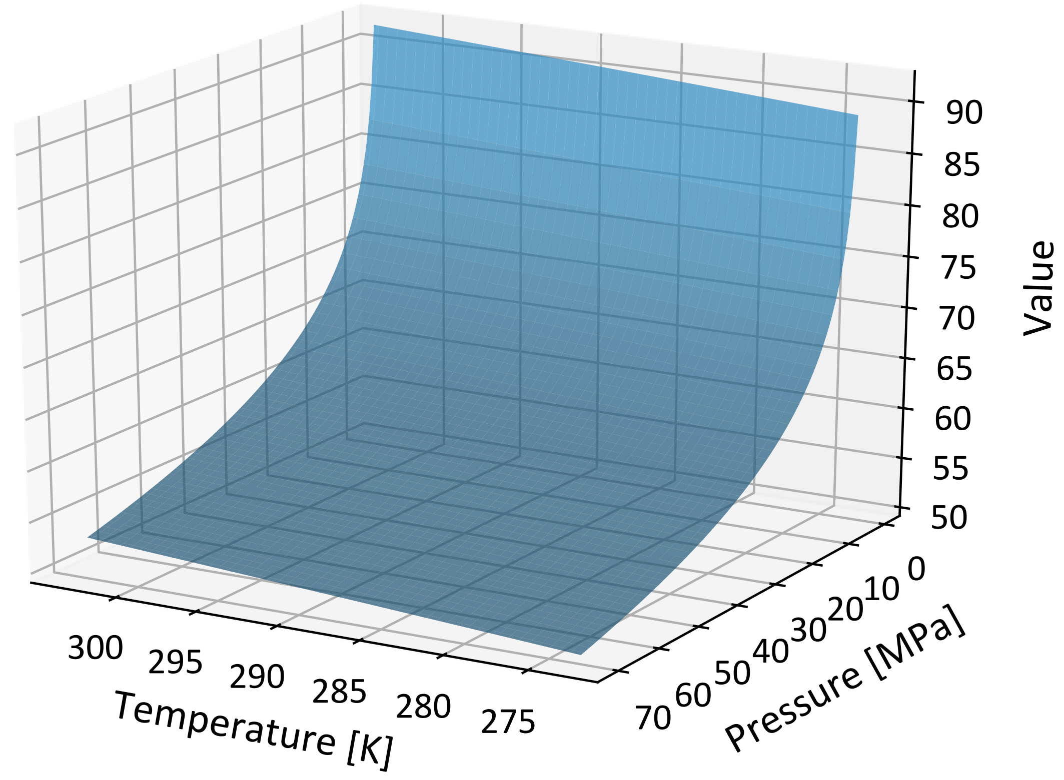
- Calculation of
    1. Density
    2. Enthalpy
    3. Entropy
    4. Viscosity
- for hydrogen and CO_2 mixtures
- Independent variables:
    1. Pressure
    2. Temperature
    3. Composition
- Basis function:
    - Taylor polynomials of order 6
- Batch sampling to avoid communication problems

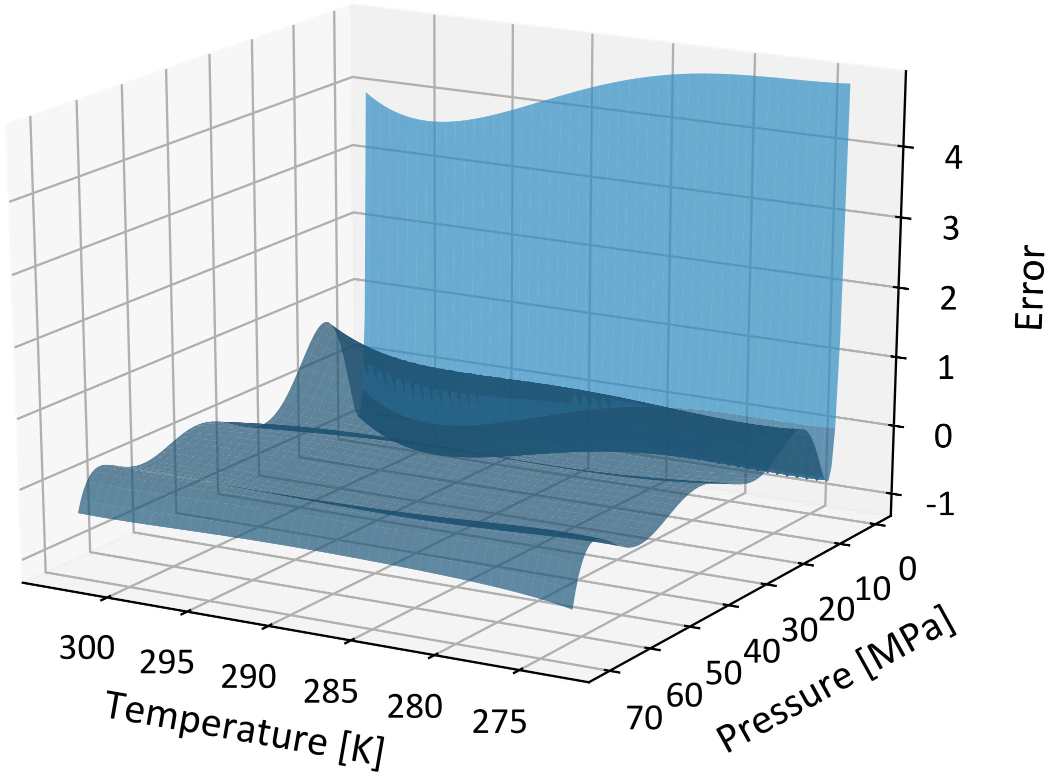
Thermodynamic property ROM
Hydrogen density





Thermodynamic property ROM
Hydrogen entropy





Conclusion

- Developed open framework for creation of reduced order models
  - Permissive license
  - No need for commercial solver/can use of-the-shelf solver
- Novelty of Consumet:
  - Incorporation of simple constraints for sampling domain reduction
  - Focus on important region to avoid complex behavior
  - Avoid that adaptive sampling routines sample unnecessary points
- Applications:
  - Optimization of chemical process and value chains, e.g. H_2 production from NG
  - Simplified thermodynamic relation for complex models, e.g fluid properties from TREND for operational model

Acknowledgements

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Link to software: https://github.com/act-elegancy/consumet
Link to blog article: https://blog.sintef.com/sintefenergy/ccs/consumet-constructor-surrogate-models-metamodels/
Journal publication in preparation