Modeling of Gas Processing Facilities Using Simscape

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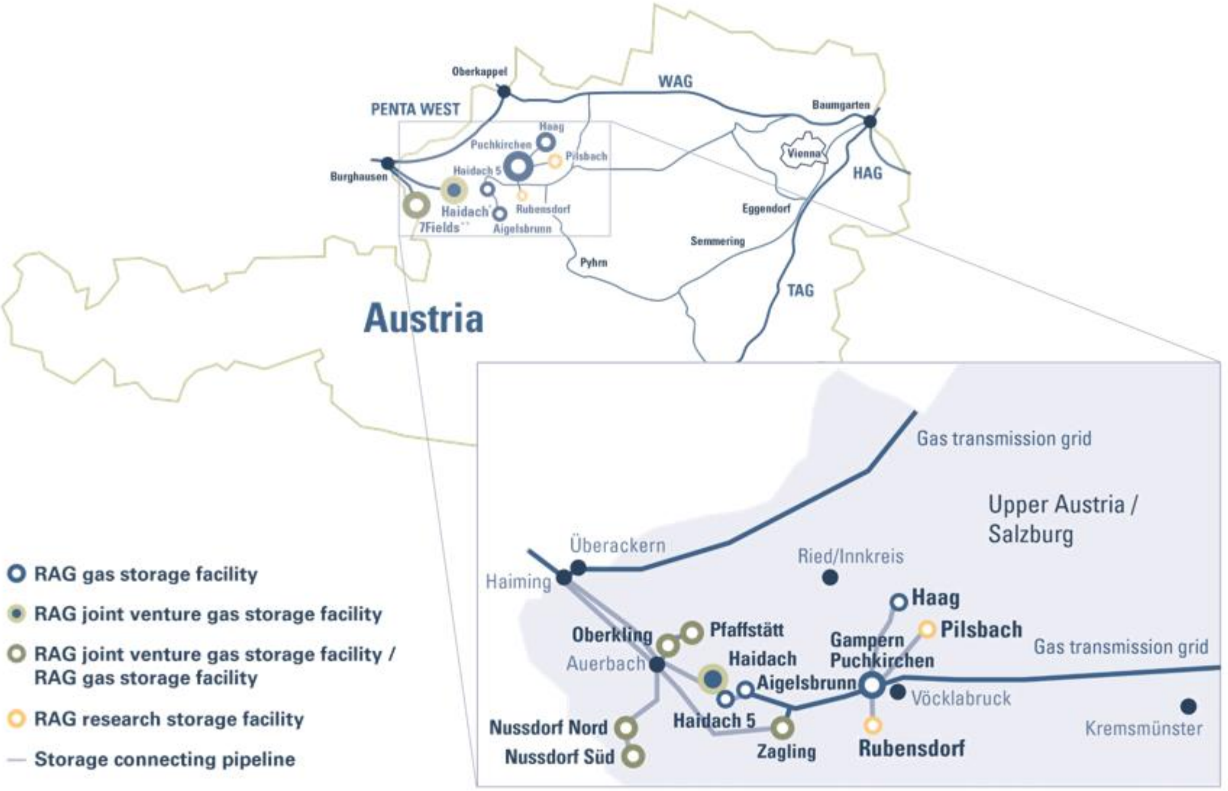
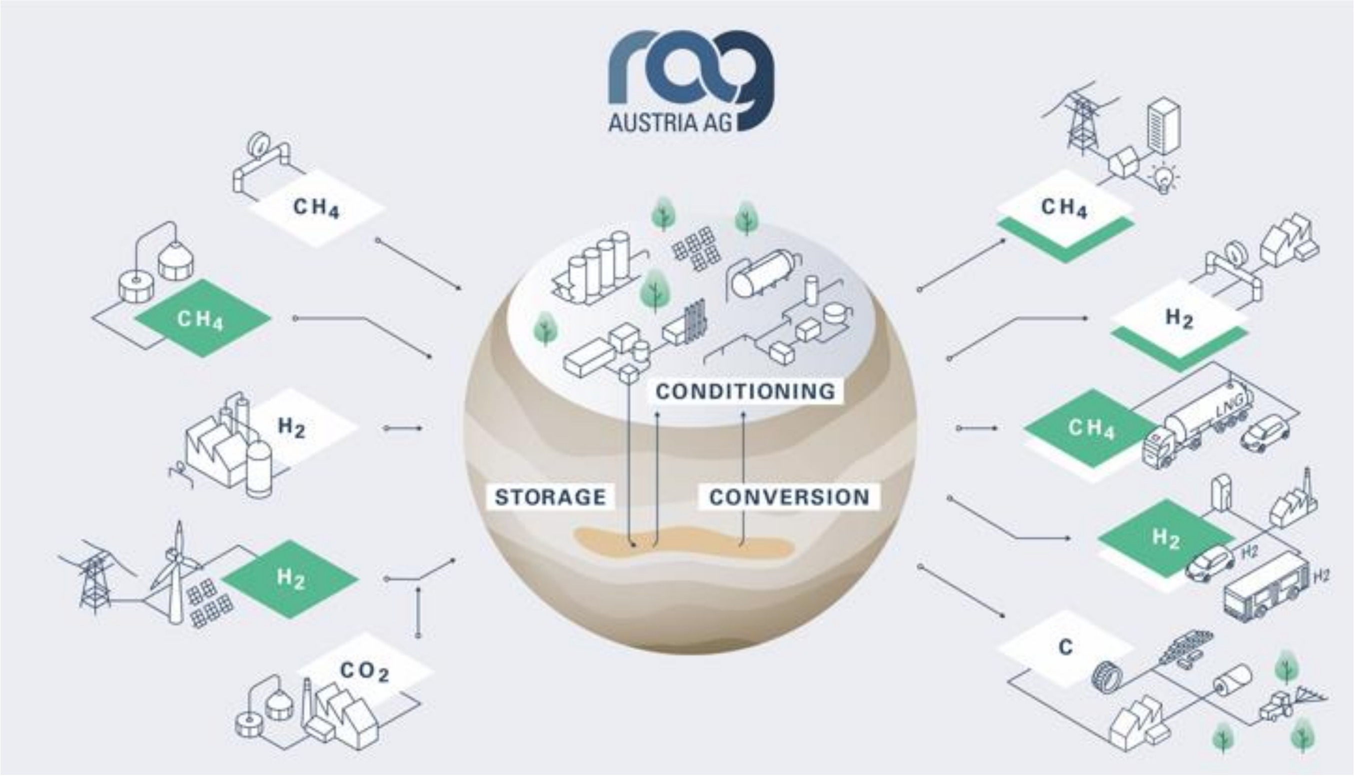
RAG Austria – Company Overview

- Founded in 1935 – **longstanding experience** in E&P operations
- Underground gas reservoirs **converted to UGS**
  → Gas / energy storage company
- **4th largest UGS operator** in Europe (6.2 bcm working gas volume)

Focus on **sustainable use of natural gas reservoirs** for underground gas storage and conversion of renewable energy to green gas and hydrogen

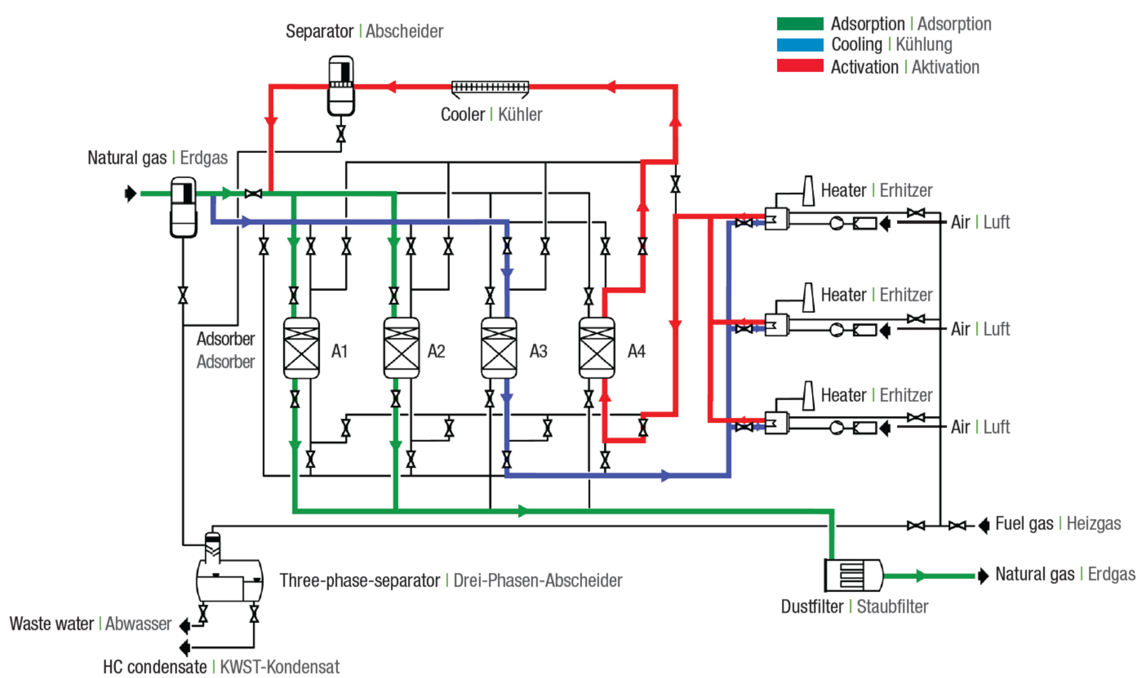
RAG – Renewables And Gas



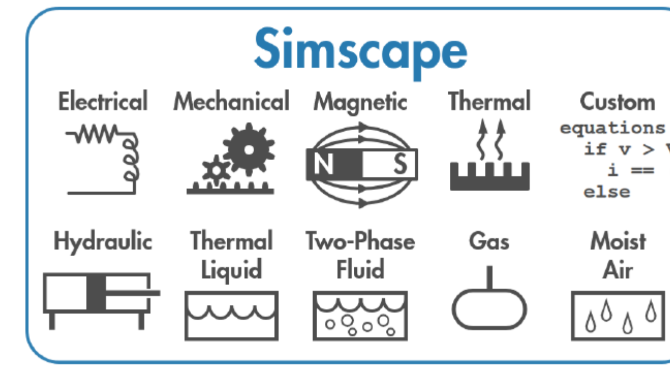


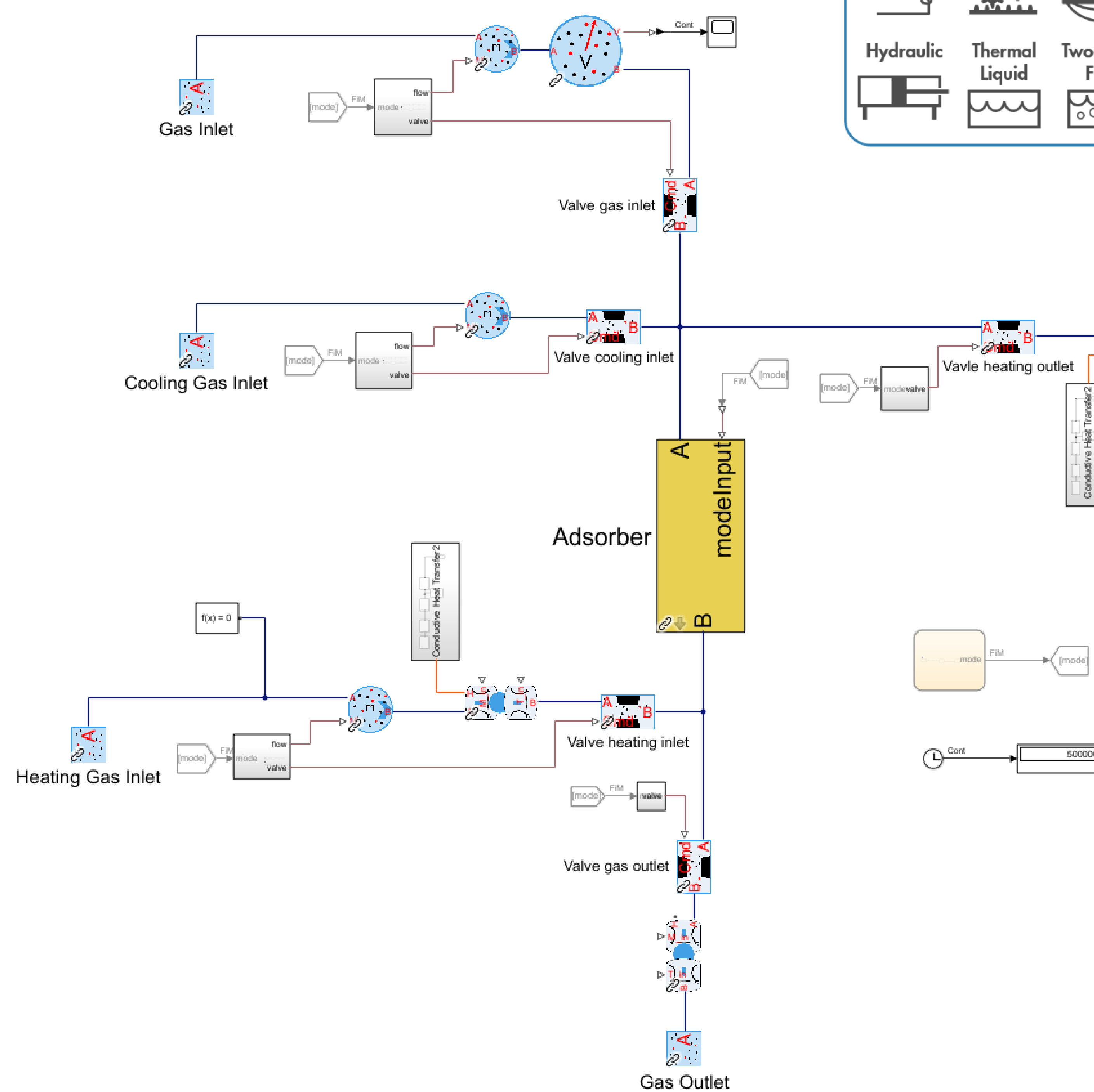
Modeling of Adsorption Dehydration Units with Simscape

- Initial motivation: evaluate Simscape for building dynamic simulation models of gas dehydration facilities (→ Digital Twins)
- Extract water vapor from gas stream by adsorption on silica gel
- Adsorption column has been set up as Custom Component in Simscape



Underground gas storage facility
with adsorption dehydration units

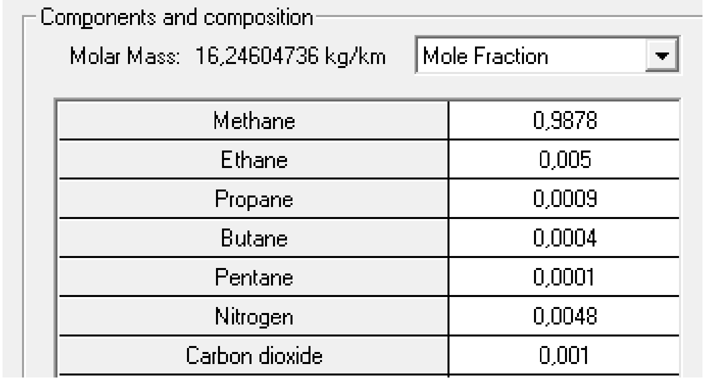




Mathematical Model for Adsorption Dehydration - Custom Component in Simscape Model

Mathematical model is based on conservation laws and thermodynamics of adsorption

- Mass conservation -> differential equation for water vapor and adsorbed water concentration
- Energy conservation -> for temperature evolution
- LDF (linear driving force) model for time dependence of adsorbed water concentration
- Experimentally validated model for adsorption isotherms
- Thermodynamic properties of gas mixture (specific enthalpy, heat capacity, thermal conductivity, viscosity etc.) are temperature and pressure dependent
- MATLAB interface to REFPROP database has been created → provides definition of gas composition in Simscape model

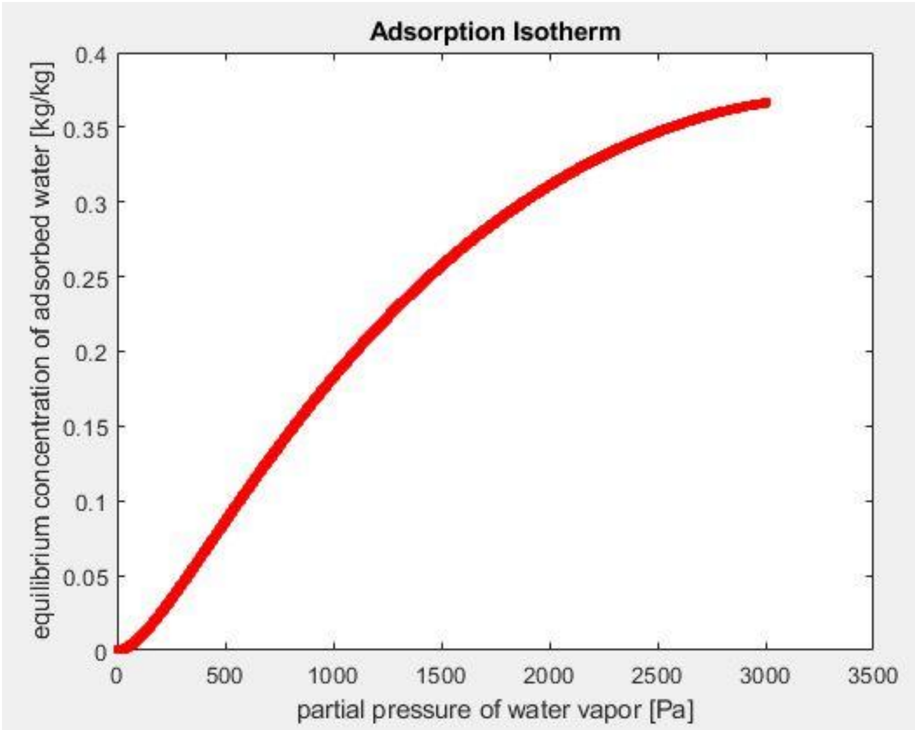

Components and composition

Molar Mass: 16,24604736 kg/km — Mole Fraction

Methane	0,9878
Ethane	0,005
Propane	0,0009
Butane	0,0004
Pentane	0,0001
Nitrogen	0,0048
Carbon dioxide	0,001

Input parameters to adsorption model

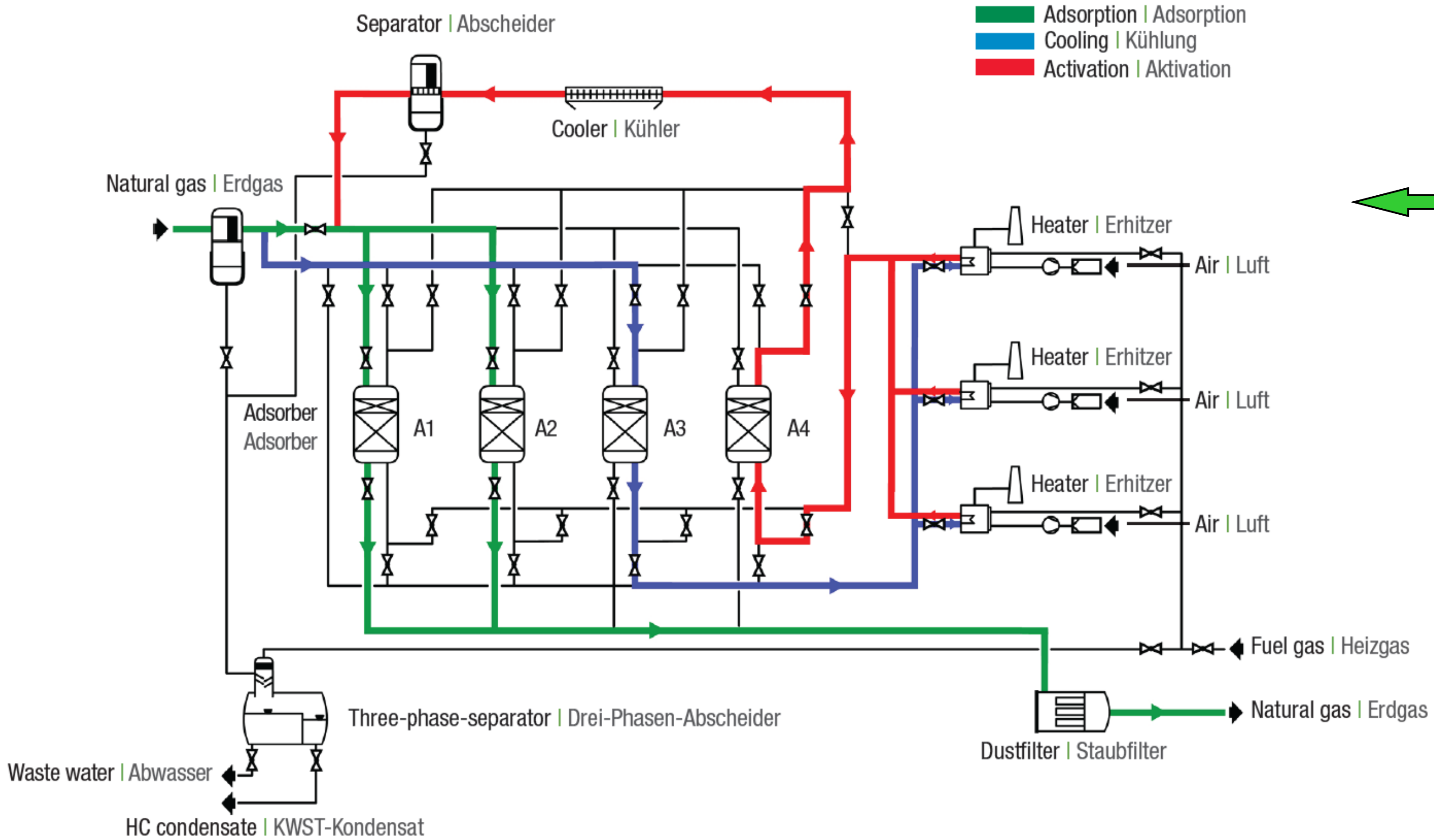
- Adsorber geometry (column height & diameter)
- Density and diameter of fixed bed particles
- Fixed bed porosity and tortuosity
- Parameters determining the adsorption isotherms



Adsorption isotherm (typical example)

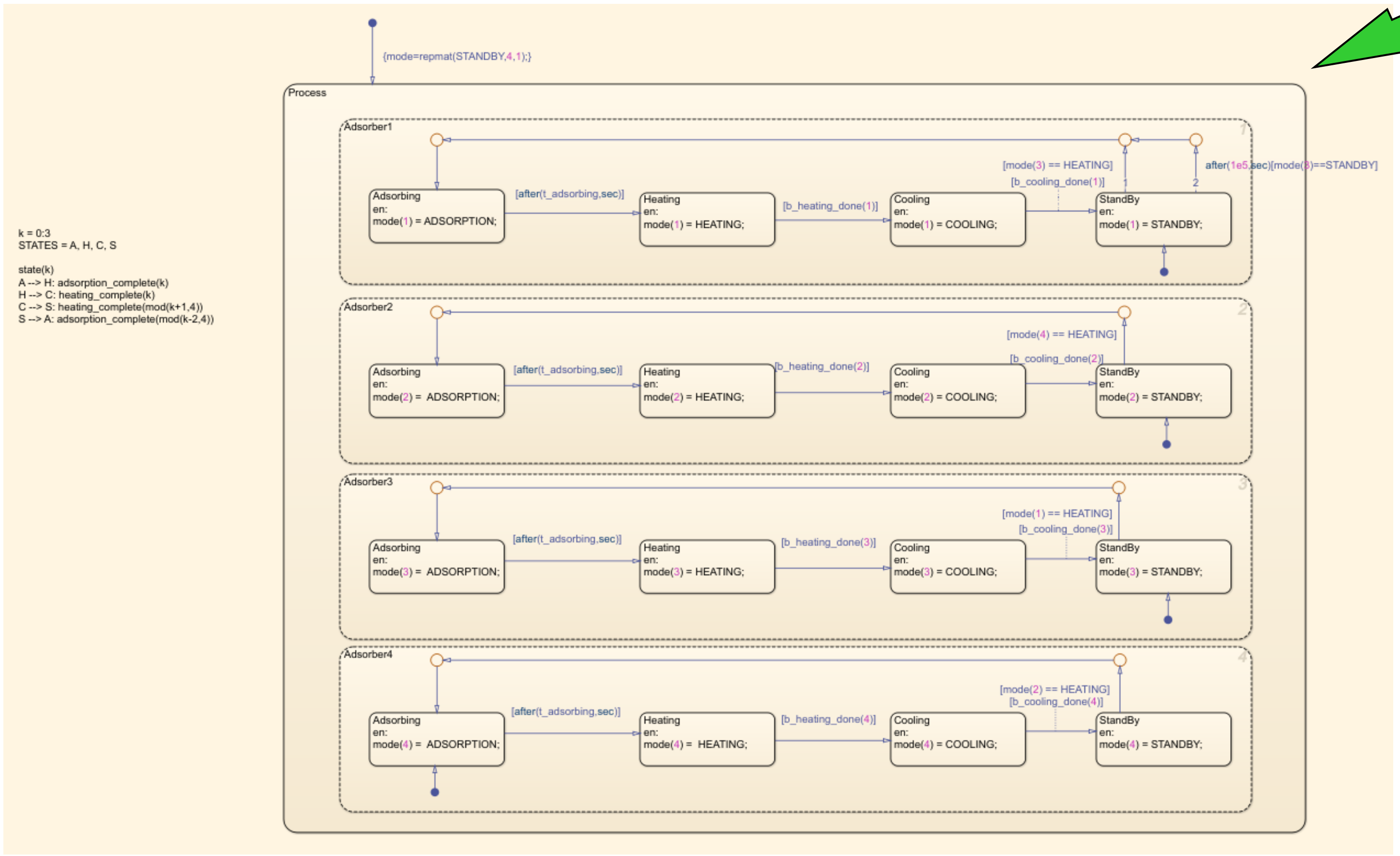
Simscape Model for Adsorption Dehydration – Switching Logic

- Four adsorbers per dehydration train (plant with four dehydration trains)

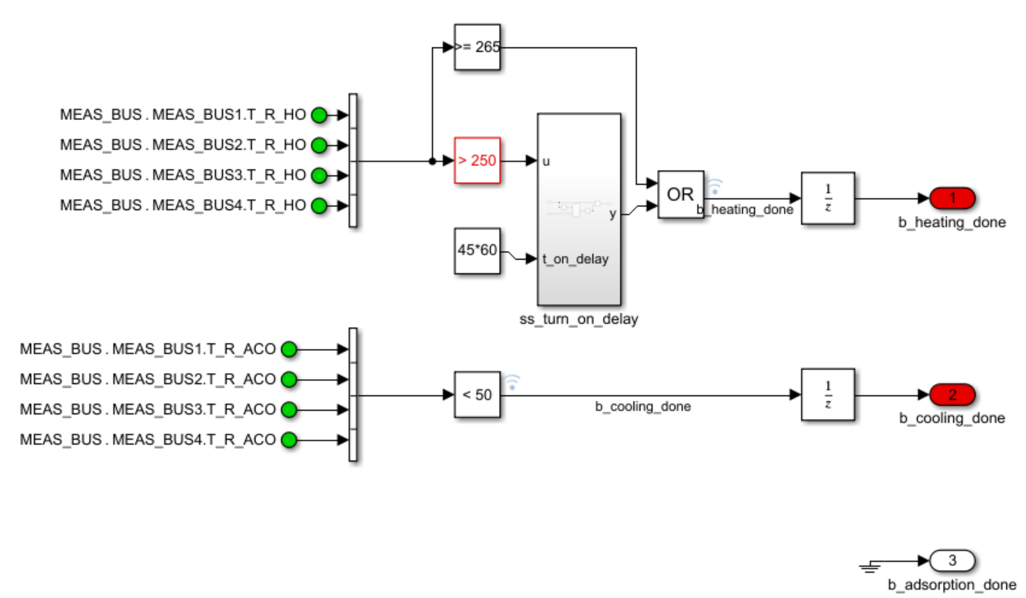


Adsorber schematics

During regeneration adsorbed water is removed from silica gel by hot gas stream (~280°C)

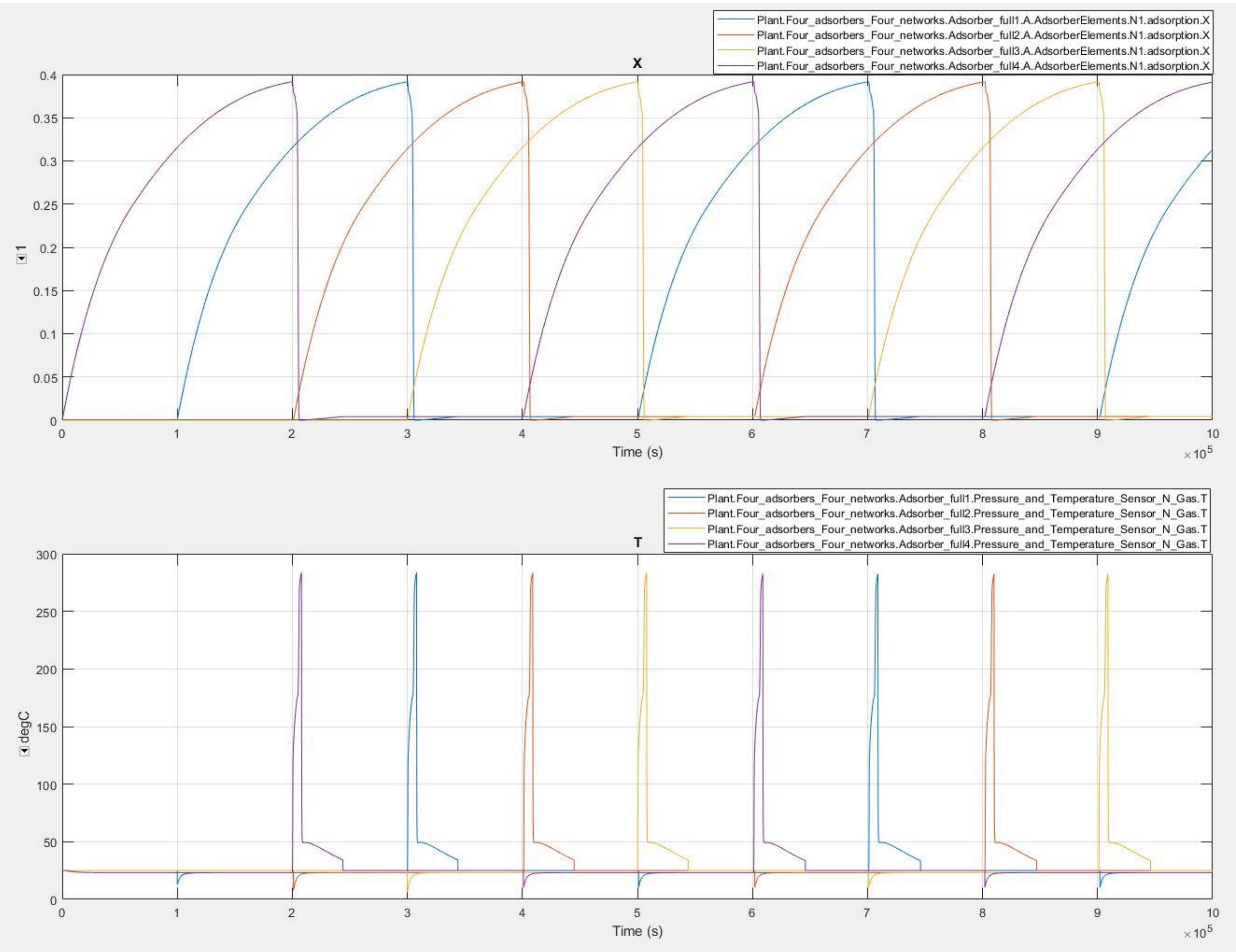


Adsorber switching logic (adsorption – regeneration – cooling) realized by **Stateflow Chart** - also based on temperature sensors at specific positions



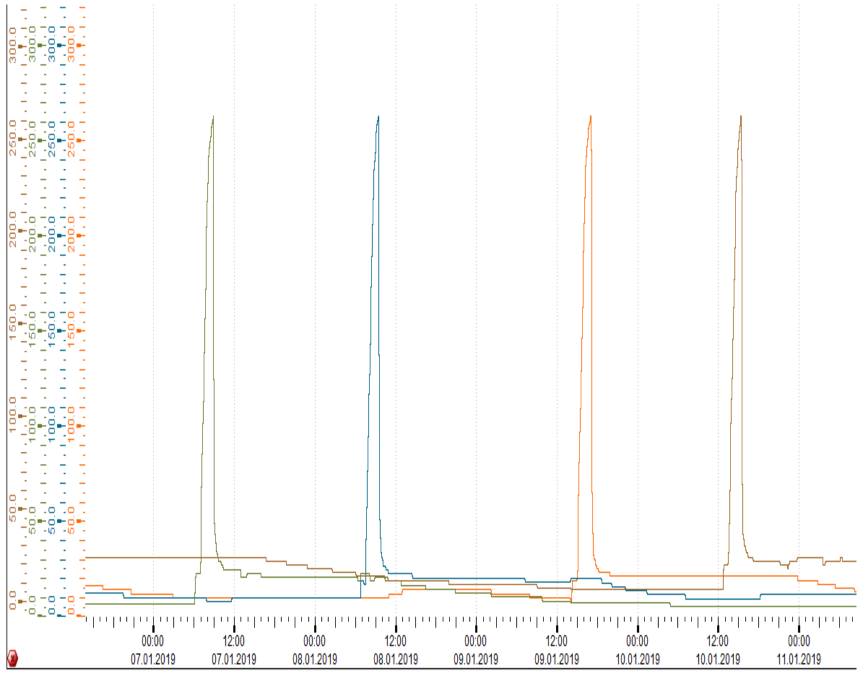
Results of „4 Adsorber Model“ and comparison with measured data

- Dynamics of cyclic adsorption and desorption process is well reproduced by Simscape model
- Simscape solver perfectly handles big temperature changes !
  (~ 250°C switching from adsorption to heating and back to cooling)



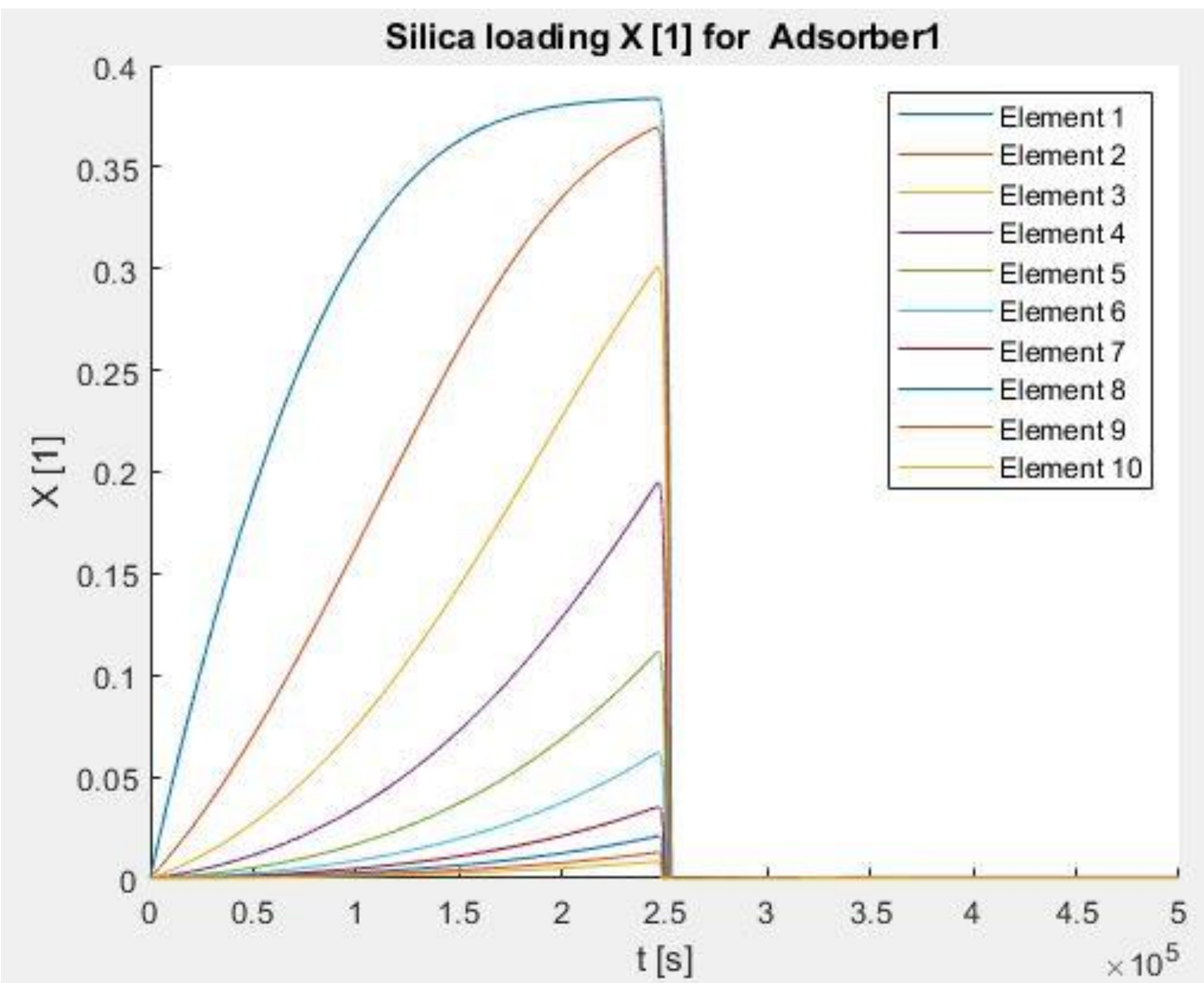
Adsorbed water [kg/kg] and simulated temperature (at sensor T4x11) as a function of time

Temperature data measured at sensor T4x11 (from SCADA system)

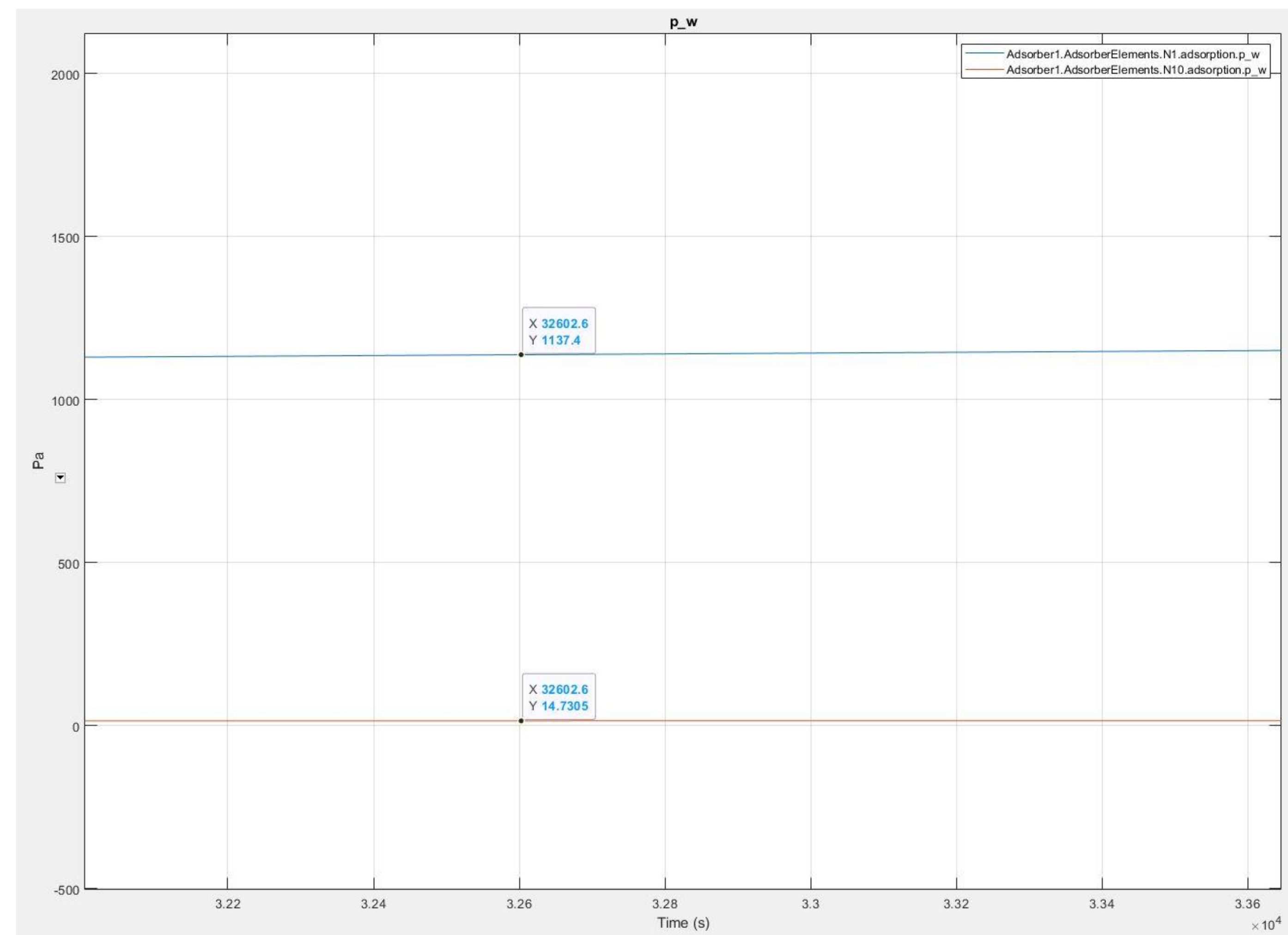


Validation of Simscape Model for Adsorption Dehydration

- Comparison with data from Jan. 2019: feed gas rate 90,000 m³/hr at 90 bar
- Calculated partial pressure of water vapor at adsorber outlet is reduced from 1130 to 15 Pa
- Partial pressure reduction corresponds to a reduction of the water dew point to -38°C
- Calculated water dew point shows very good agreement with measured dew point data



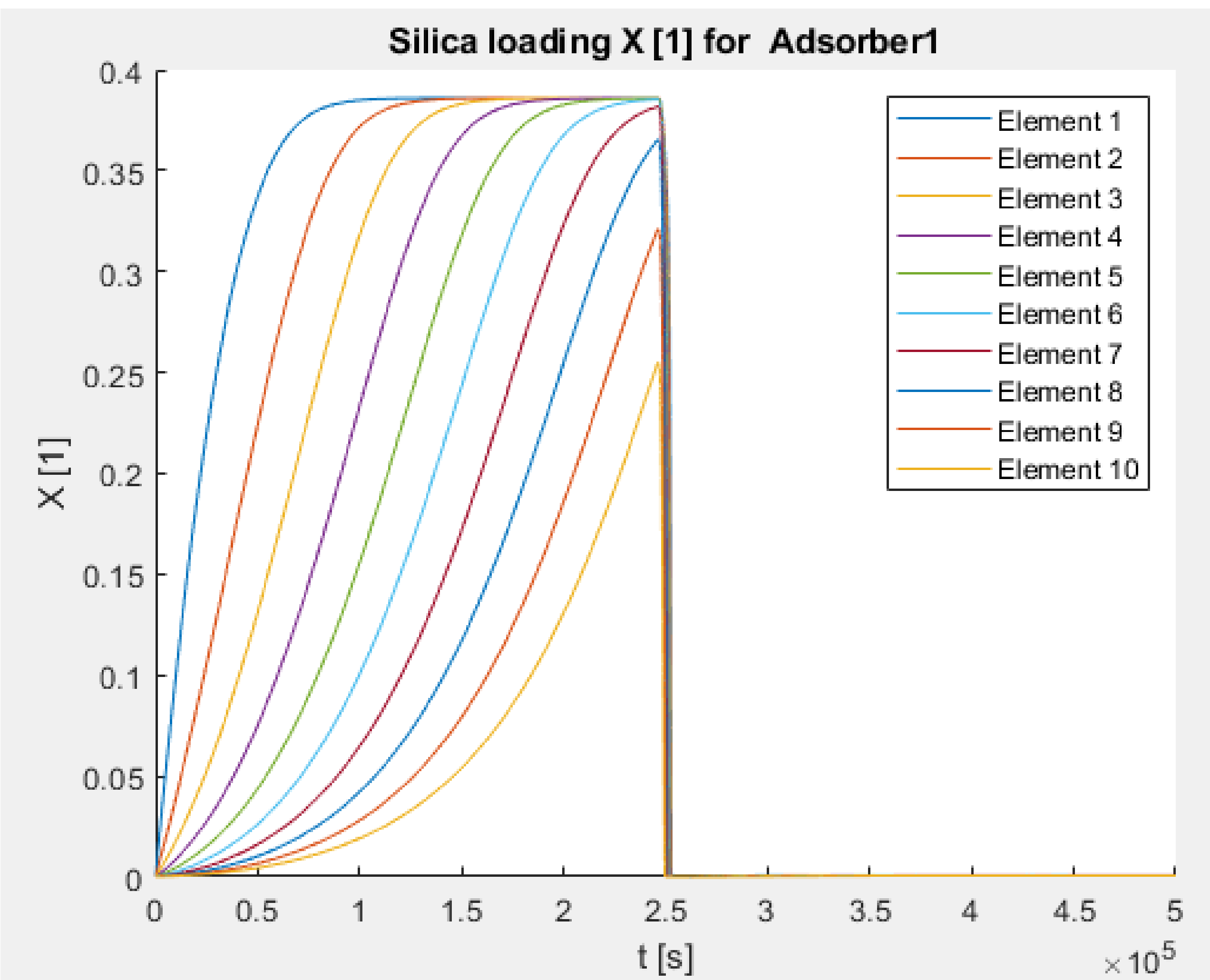
Adsorbed water [kg/kg] as a function of position and time
(switching from adsorption to regeneration after 68 hrs.)



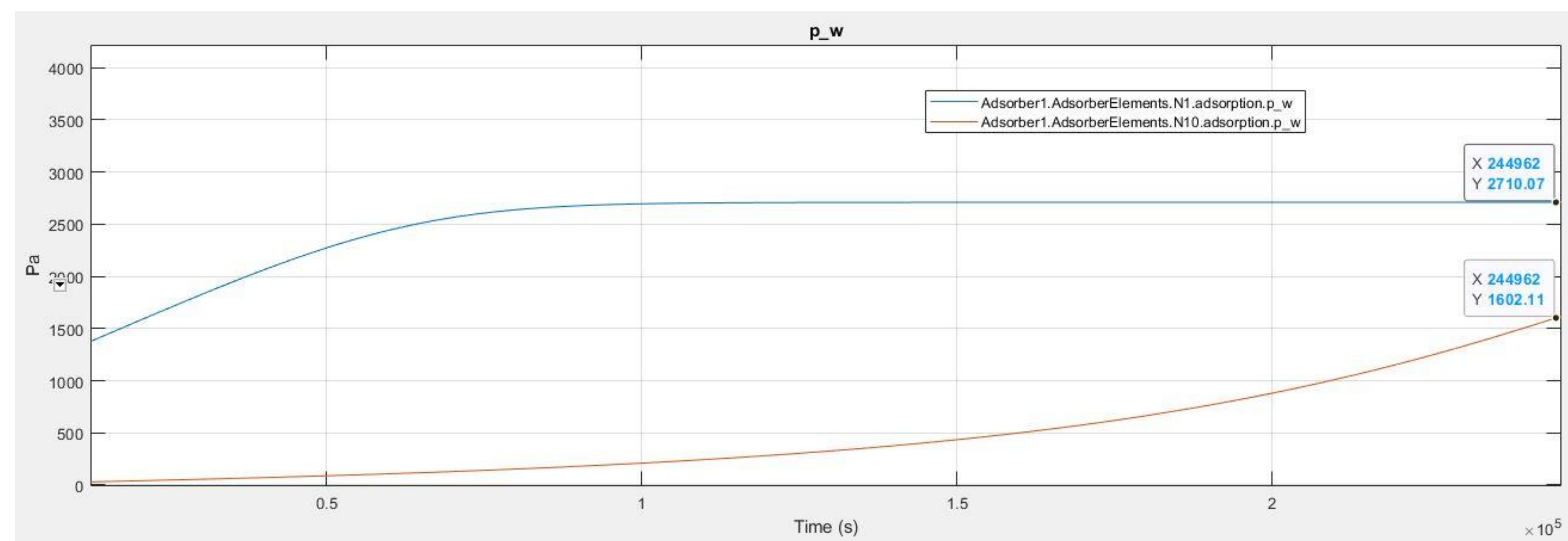
Water vapor partial pressure [Pa] as a function of time
(adsorber inlet … blue,
adsorber outlet … red)

Evaluation of alternative scenarios: 310,000 m³/hr per adsorption train, at 55 bar (2 adsorbers in parallel at 155,000 m³/hr each)

- Adsorber reaches saturation over almost entire length
- Water vapor partial pressure at adsorber outlet goes up to 1600 Pa towards end of adsorption phase → corresponding to a dew point of +14 °C
- Dew point specification will not be met (- 8 °C at 70 bar) → Adsorption cycle time needs to be reduced for this scenario !



Adsorbed water [kg/kg] along adsorber as a function of time

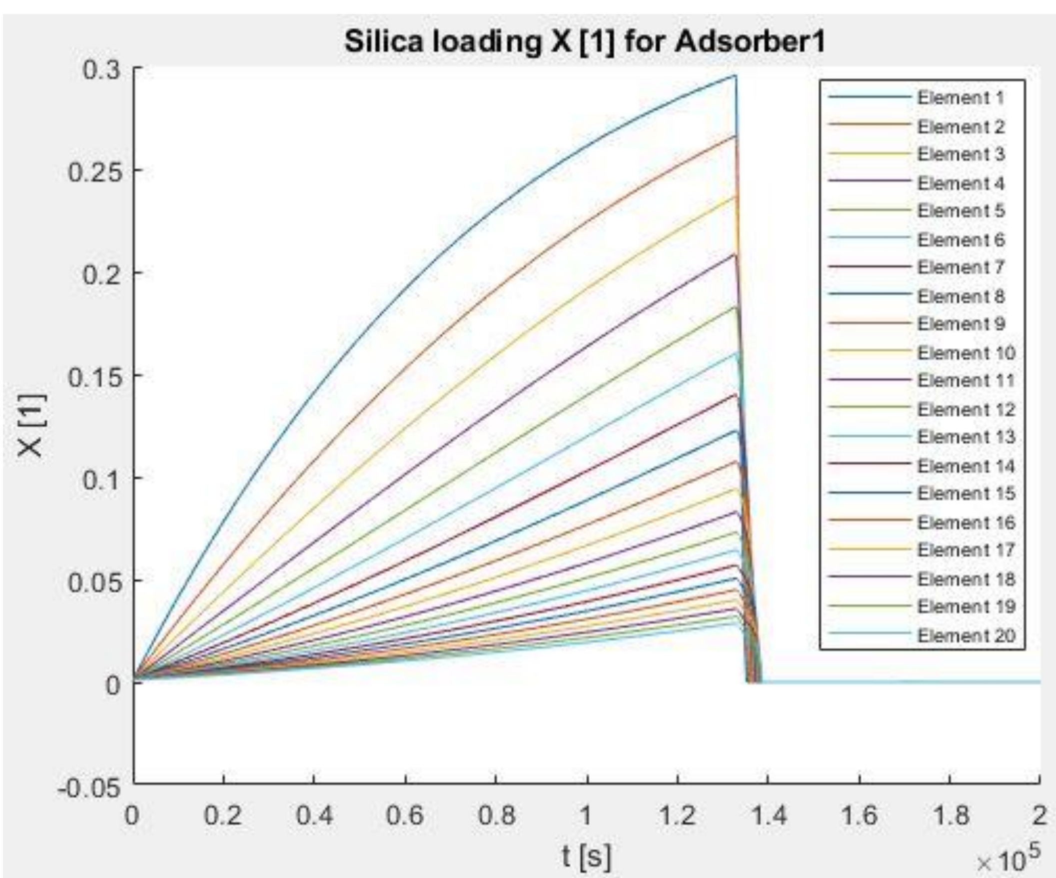


Water vapor partial pressure [Pa] as a function of time (adsorber inlet … blue, adsorber outlet … red)

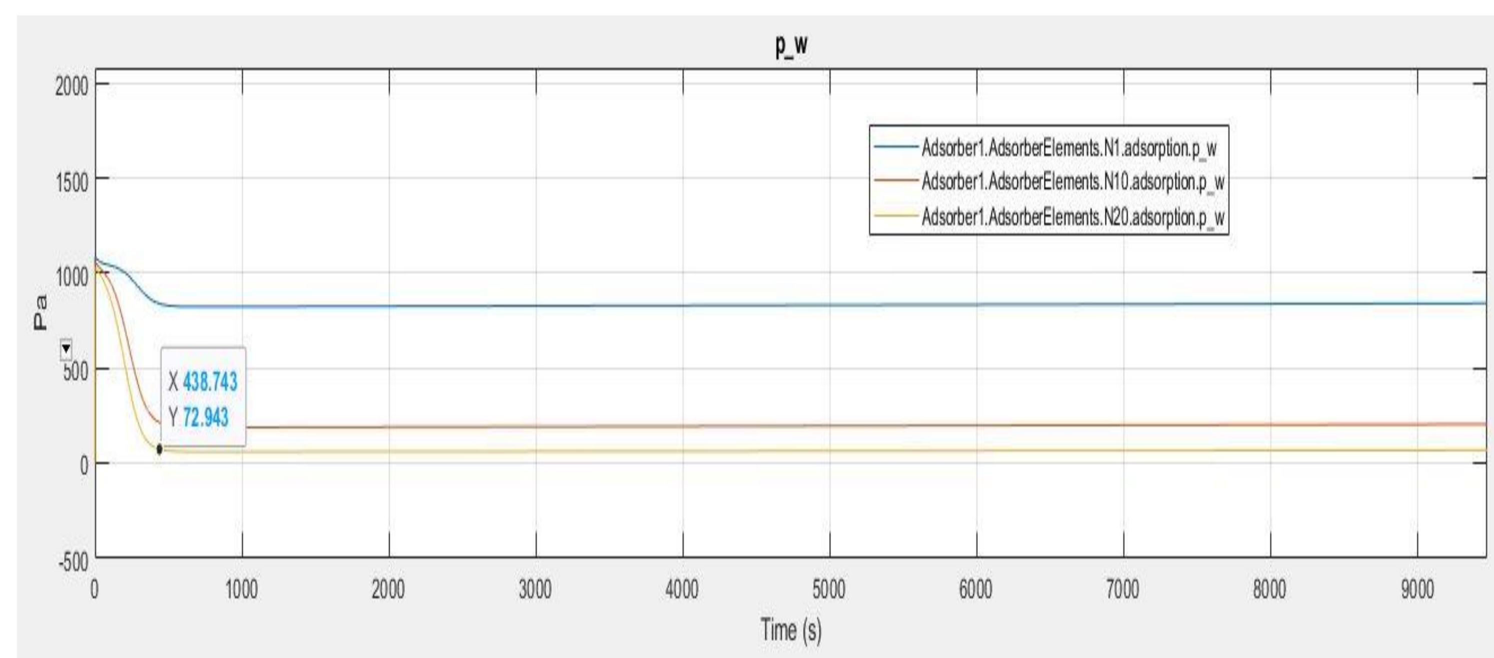
Hydrogen content in gas stream

- Adsorption dehydration model applied to **hydrogen storage research facility**
- Hydrogen in injection gas being generated by **water electrolysis** unit
- ~10 mol-% H_2 content in produced gas

- Comparison with data from July 2020: 2000 m³/hr at 35 bar
- Calculated partial pressure of water vapor at adsorber outlet is reduced to 72 Pa
- Partial pressure reduction corresponds to a reduction of the water dew point to -24°C
- Calculated water dew point shows very good agreement with measured dew point data (-23.4°C)



Adsorbed water [kg/kg] along adsorber as a function of time



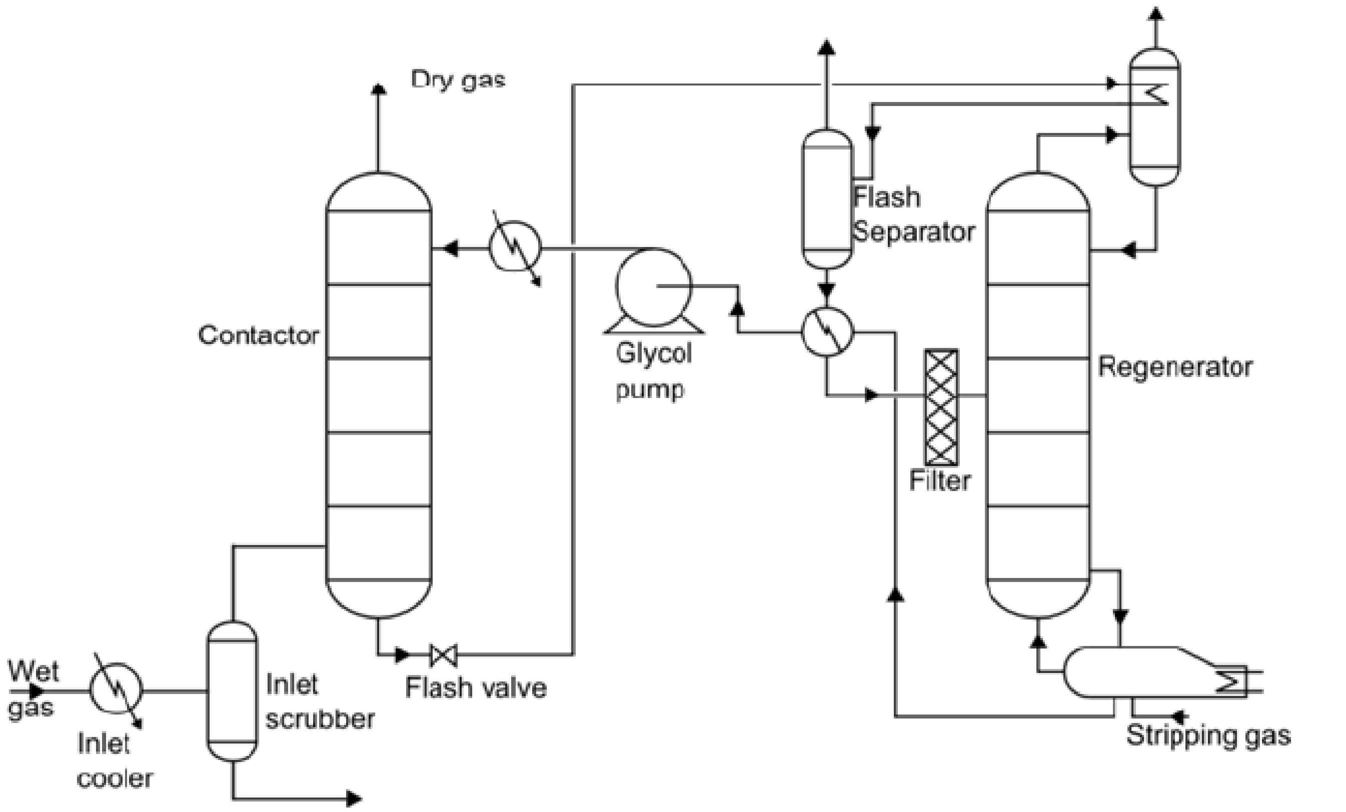
Water vapor partial pressure [Pa] as a function of time

Applications of Simscape Adsorption Dehydration Model

- Capacity estimation in engineering of adsorption dehydration plants
- Evaluation of energy consumption at various operating modes
- Estimation of water break-through times
- Optimization of cycle times (duration of adsorption, regeneration, cooling)
- Determination of achievable dew point
- Impact of hydrogen content in gas stream on adsorption process

Modeling of Glycol Dehydration Units with Simscape

Absorption columns



Underground gas storage facility with glycol dehydration units

Typical glycol dehydration schematics → water vapor is absorbed by a circulating glycol stream

Mathematical Model for Glycol Dehydration - programmed as a Custom Component in Simscape Model

Mathematical model is based on conservation laws and thermodynamics of vapor / liquid equilibria

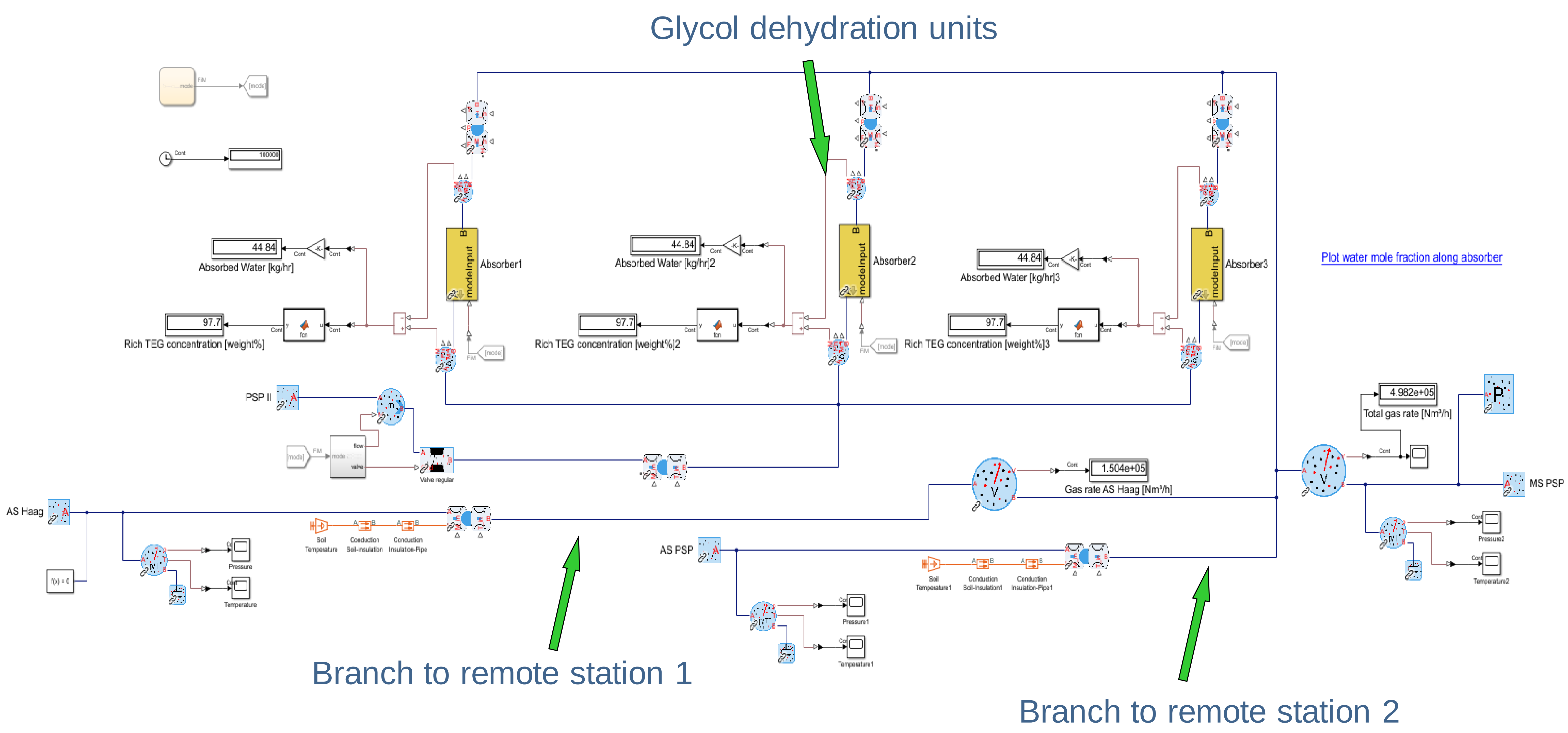
- Mass conservation
- Energy conservation
- Phase equilibria of water vapor and glycol
- Glycol density and activity coefficients
- Thermodynamic properties of gas mixture (specific enthalpy, heat capacity, thermal conductivity, viscosity etc.) are temperature and pressure dependent
- MATLAB interface to REFPROP database to obtain thermodynamic properties of gas mixture

Input parameters to absorption model

- Absorber geometry (column height & diameter)
- Feed gas rate
- Glycol circulation rate
- Reboiler temperature and pressure

Simscape Model of UGS Plant with Glycol Dehydration Units

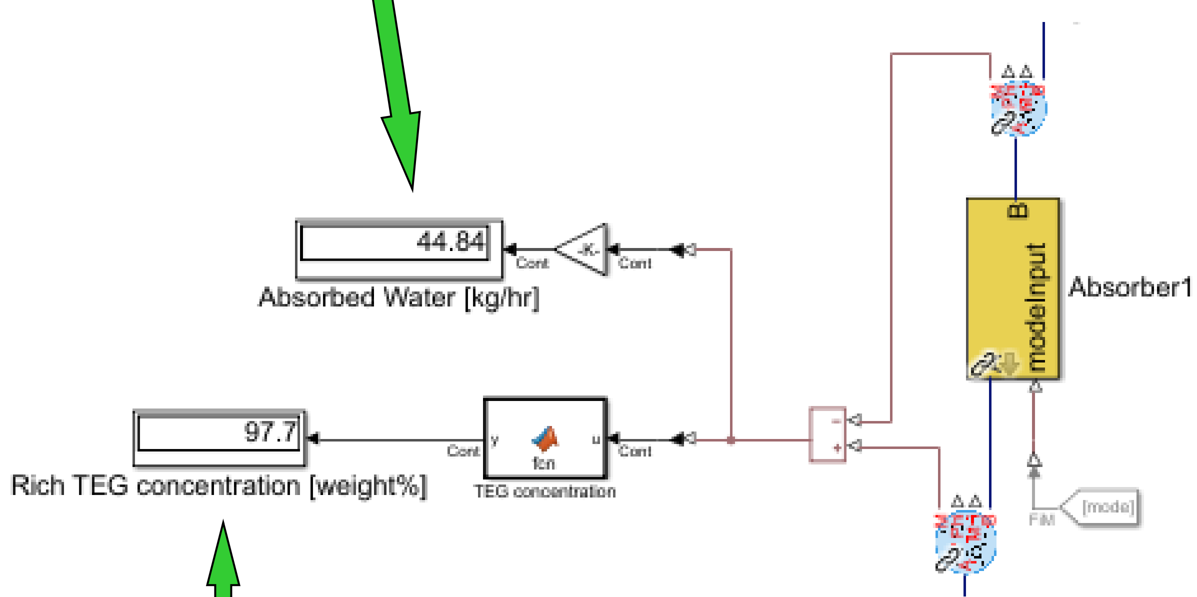
- **Central station plus two remote stations**



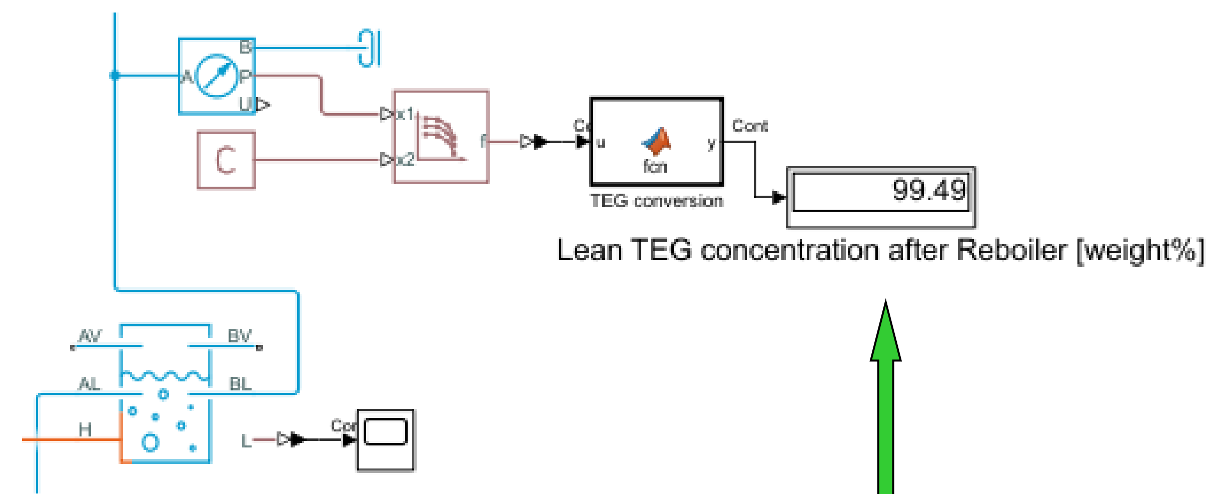
Simscape Glycol Dehydration Model – Details

- Display of vital process parameters (absorbed water, glycol concentration at absorber and reboiler outlet, gas rates, etc.)
- Simscape offers a variety of customizable display options

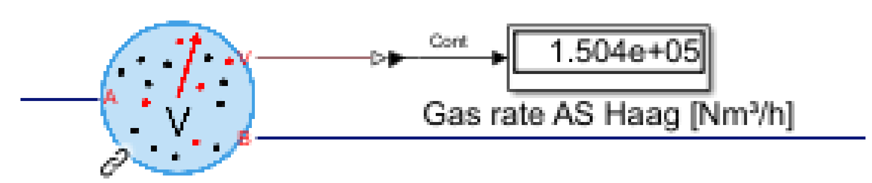
Absorbed water [kg/hr]

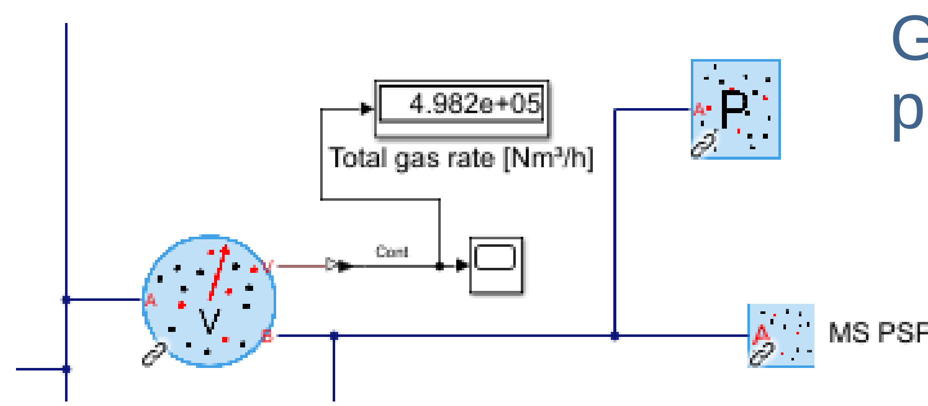


TEG concentration at absorber outlet [weight %]



TEG concentration at reboiler outlet [weight %]

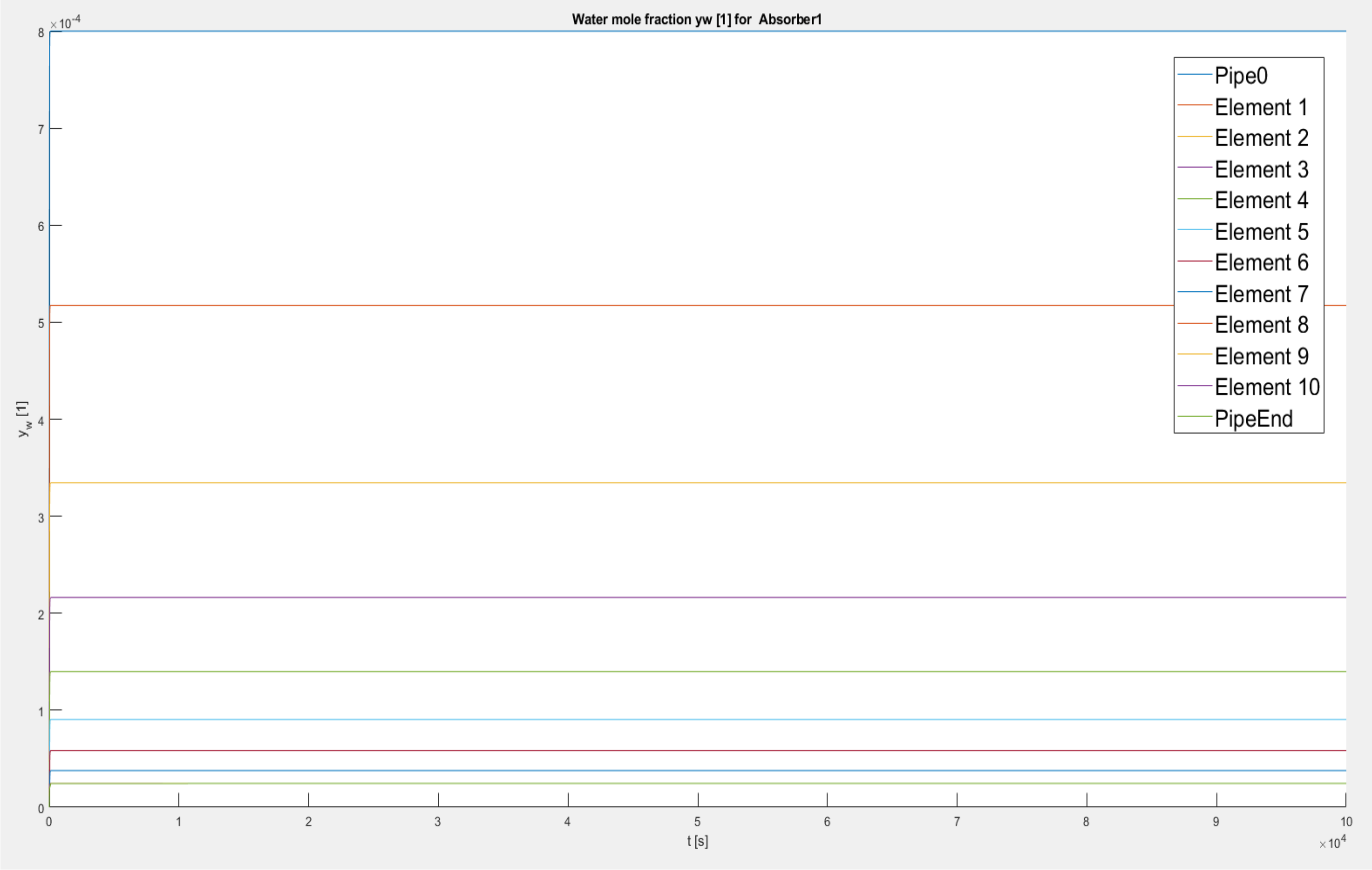


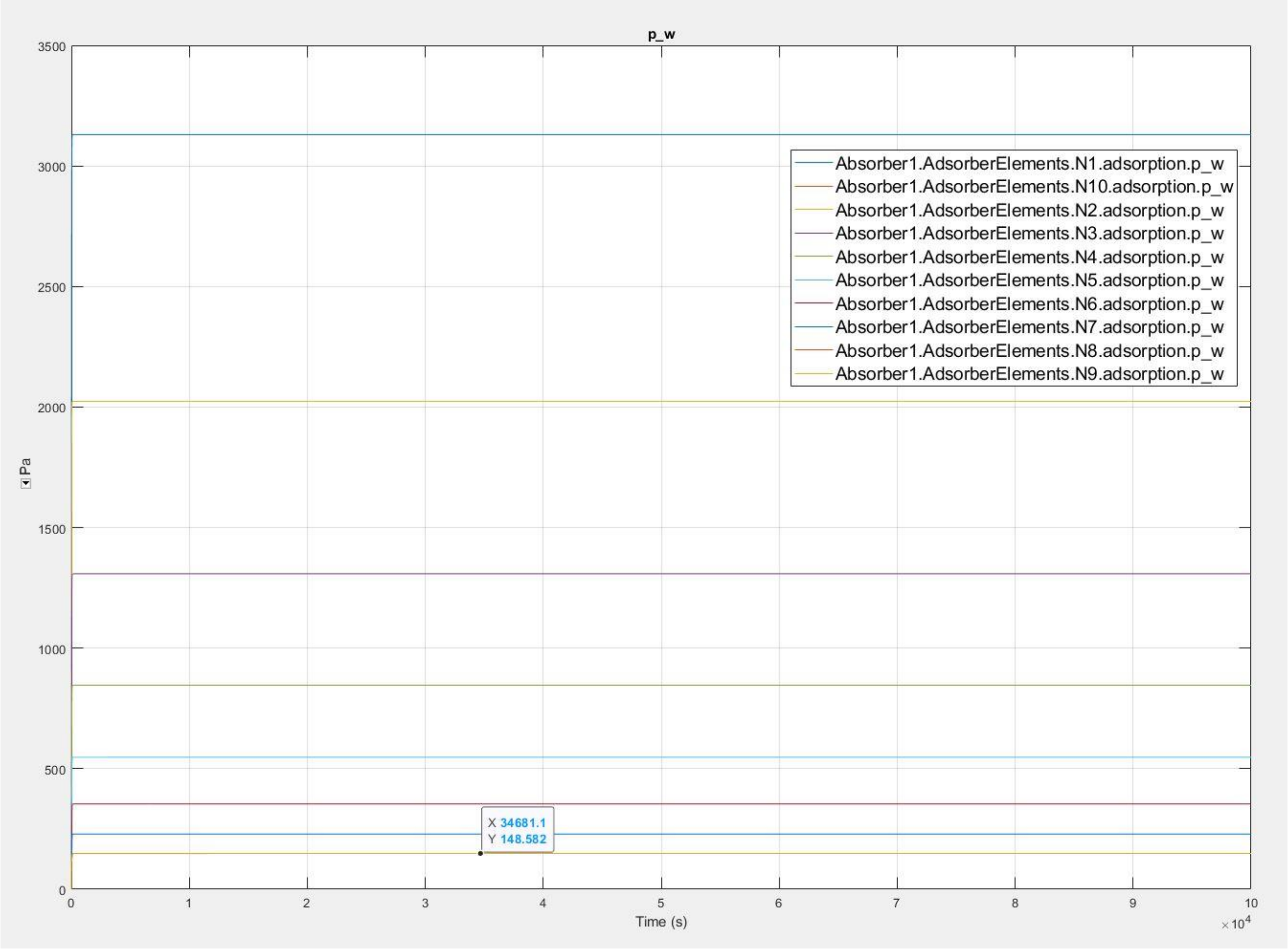


Gas rates at different positions of the plant [m³/hr]

Validation of Simscape Model for Glycol Dehydration

- Comparison with data from Jan. 8th, 2021: total gas production rate of 500,000 m^3/hr
- Model input data: pressure and temperatures at wellheads and at transfer station
- Calculated partial pressure of water vapor at absorber outlet is reduced to 149 Pa
- Partial pressure reduction corresponds to a reduction of the **water dew point** to -16 °C
- Calculated gas production rate and dew point show very good agreement with measured data
- Calculated glycol (TEG) concentration at absorber outlet: 97,7 [weight %]



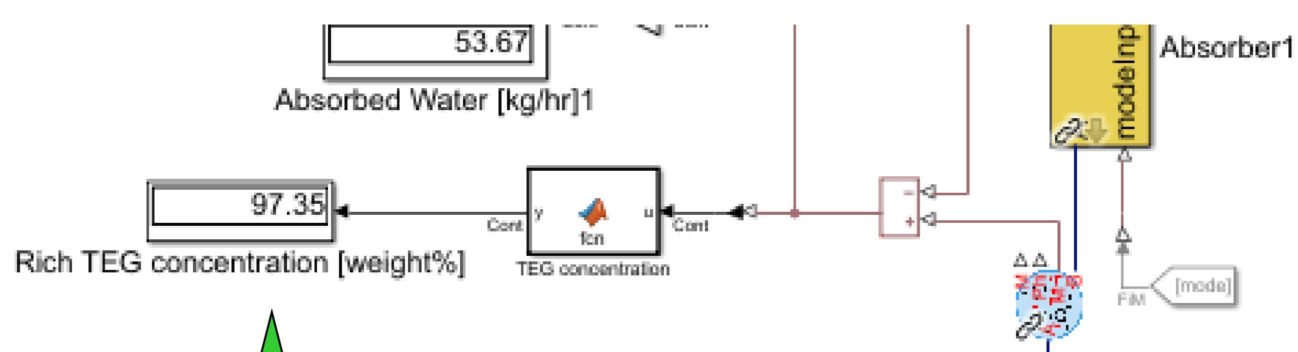


Water vapor concentration [mol fraction] and water vapor partial pressure [Pa] along the absorber column (using 10 absorber segments)

Glycol dehydration: Results with hydrogen content in gas stream

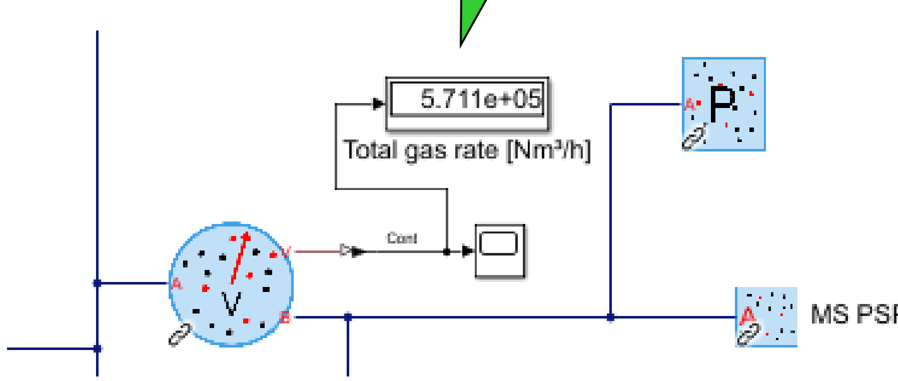
- Effects of 20 mol-% hydrogen content (at same pressures and temperatures as in model without H_2):
- Total gas rate increases from 500,000 to 571,000 m³/hr due to lower gas density
- TEG concentration at absorber outlet is decreased from 97,7 to 97,3 [weight %]
- Absorbed water increases from 45 to 53 kg/hr (at 100% water saturated gas)

Absorbed water [kg/hr]



TEG concentration at absorber outlet [weight %]

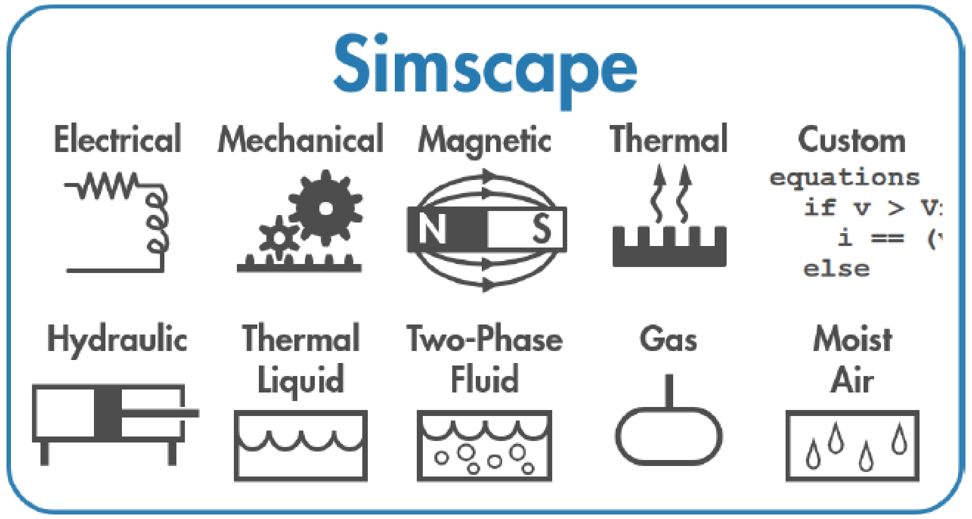
Total gas rate [m³/hr]



Applications of Simscape Glycol Dehydration Model

- Estimation of dehydration capacity in engineering of glycol dehydration units
- Impact of feed gas rate, glycol circulation rate und glycol concentration on water dew point
- Impact of reboiler pressure and temperature on achievable glycol concentration at the regeneration outlet
- Optimization of certain process parameters to comply with dew point specifications
- Evaluation of energy consumption at different operating conditions
- Effects of hydrogen content in gas stream on the absorption process and on dehydration capacity

Summary & conclusions



- Simscape has extensive library of components from different physical domains to build complex models
- Custom Component functionalities in Simscape can be applied to set up new components for modeling gas processing facilities
(once the mathematical model has been established)
- Powerful solver – can handle big changes in input parameters during simulation
- Input parameters (e.g. pressure at wellhead) can be fed into Simscape model from external sources (SCADA system) → build Digital Twins
- Simscape is valuable tool for planning and optimization purposes of gas processing facilities
- Looking forward to new applications in hydrogen technology & renewables

Thank you !

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