ESA modelling and cycle design

WP 2 and WP 5

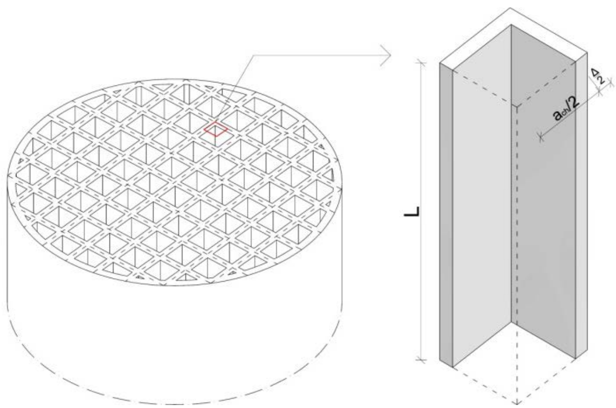
University of Belgrade

MATESA Dissemination day, Oslo 16.6.2016

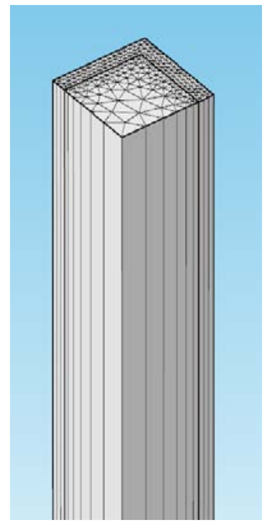
Motivation

- Develop rigorous 3D models (CFD) to understand the processes, examine the influence of conditions / parameters and have a basis for model reduction
- Develop simplified 1D models for cycle simulations, with model parameters estimated based on 3D simulations
- Design ESA cycle that will satisfy demands for high Purity (P>95%) and Recovery (R>90%)
- Analyze electric energy consumption and relations to P and R
- Analyze options to reduce the electric power consumption by means of heat recovery and use of existing thermal power
- Relate the results to experimental data

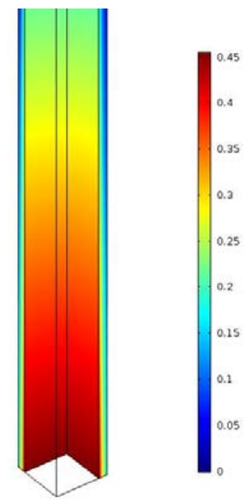
3D modelling



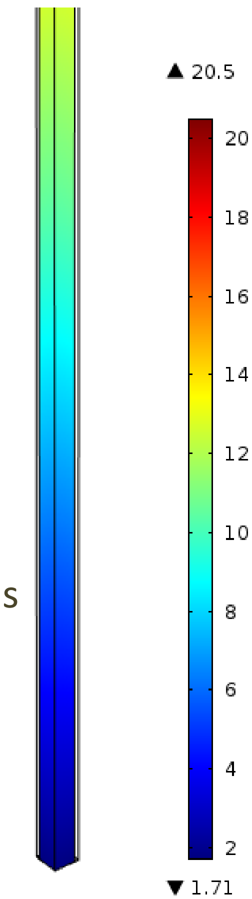
Monolith geometry and ¼ of a channel for 3D modeling



Model mesh

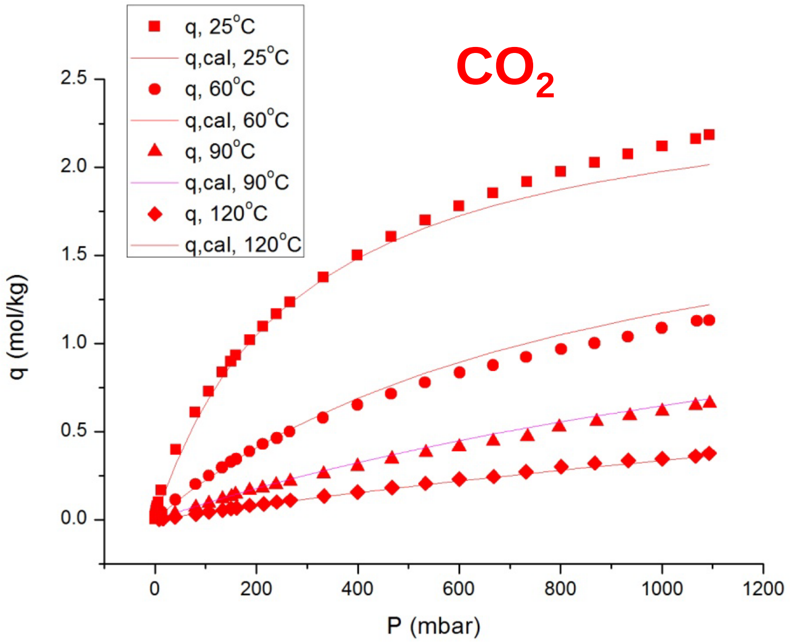


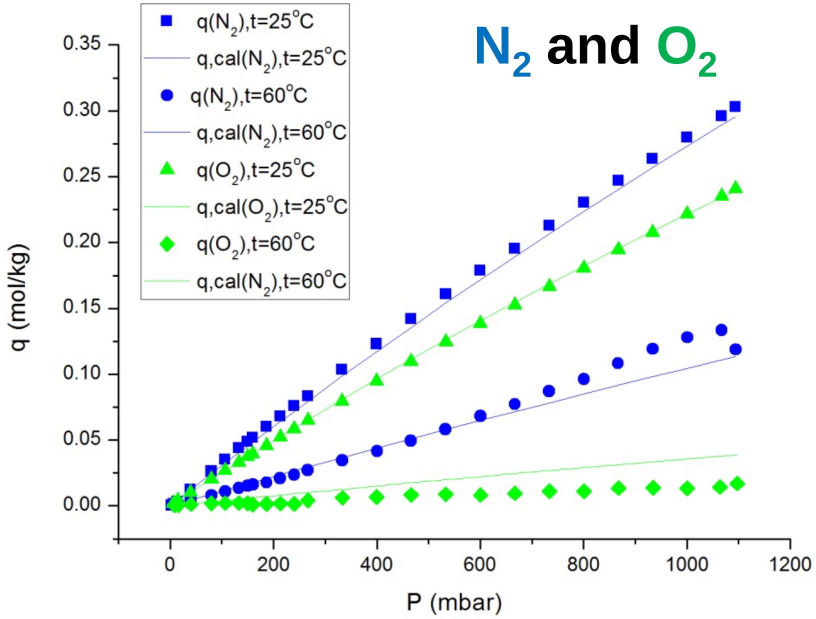
Adsorption and desorption simulations



- Detailed 3D modeling of adsorption / desorption in single channel of the monolith in Comsol Multiphysics
- Main model features: non-stationary multicomponent mass transfer (diffusion), competitive adsorption isotherms, laminar flow momentum balance and Joule heating

Adsorption isotherms

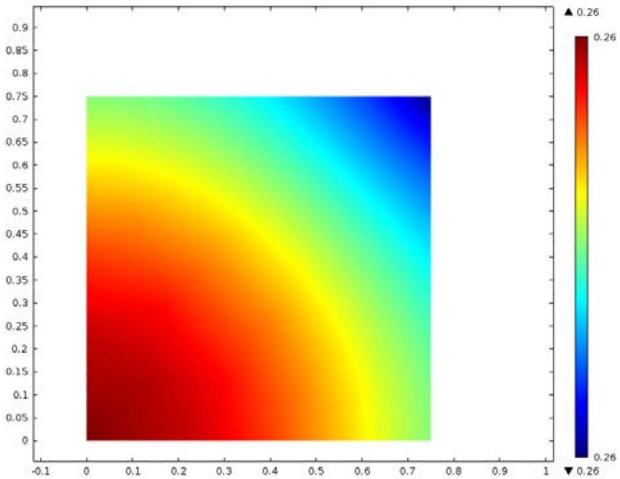




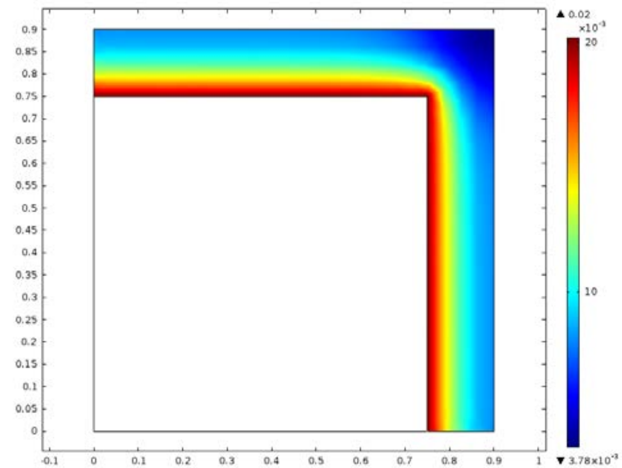
- Competitive adsorption – Langmuir model
- Based on experimental masurements for zeolite-carbon monolith (WP-4)
- Temperature dependence of q_0 and b obtained

$$q_i = q_{0,i} \frac{b_i P_i}{1 + \sum_{j=1}^{N} b_j P_j}$$

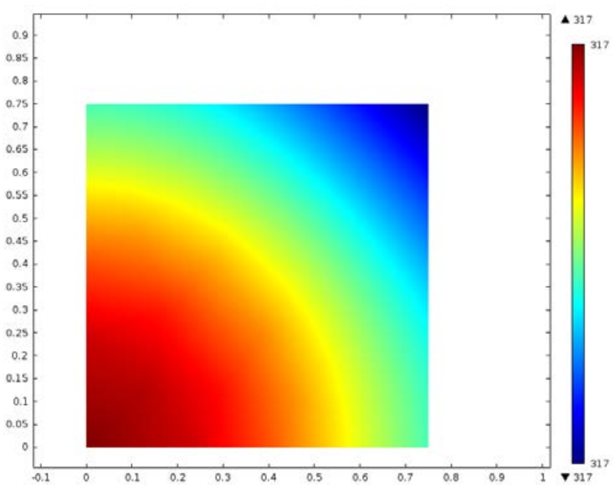
3D simulations - results



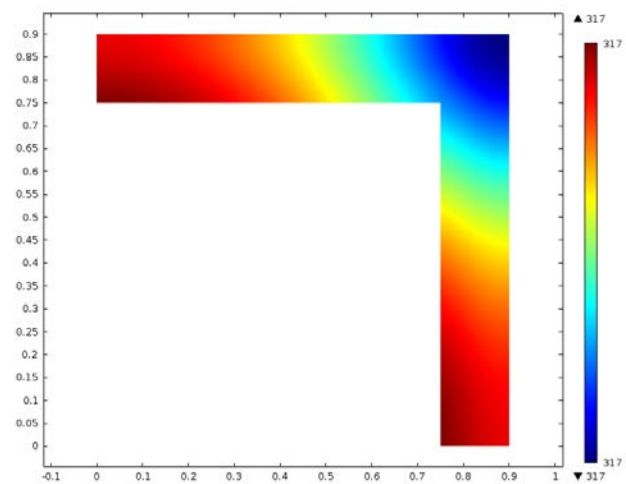
CO_2 concentration in gas (channel) at certain position and time



CO_2 concentration in solid (adsorbent) at certain position and time



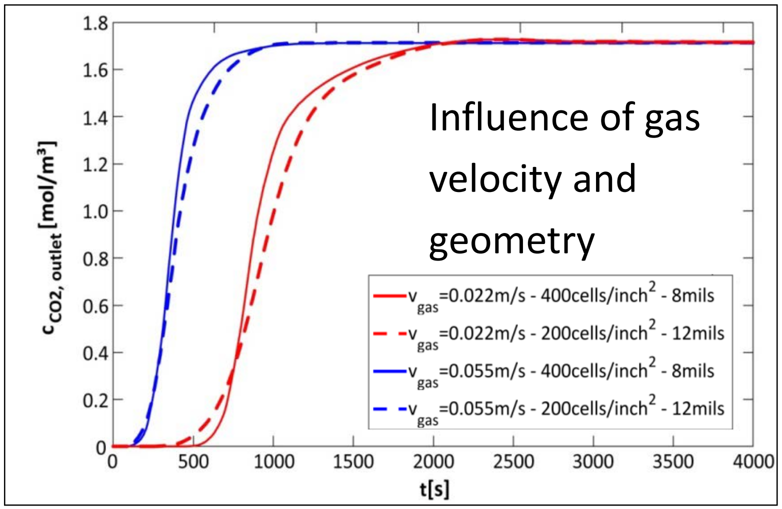
Gas temperature at certain position and time

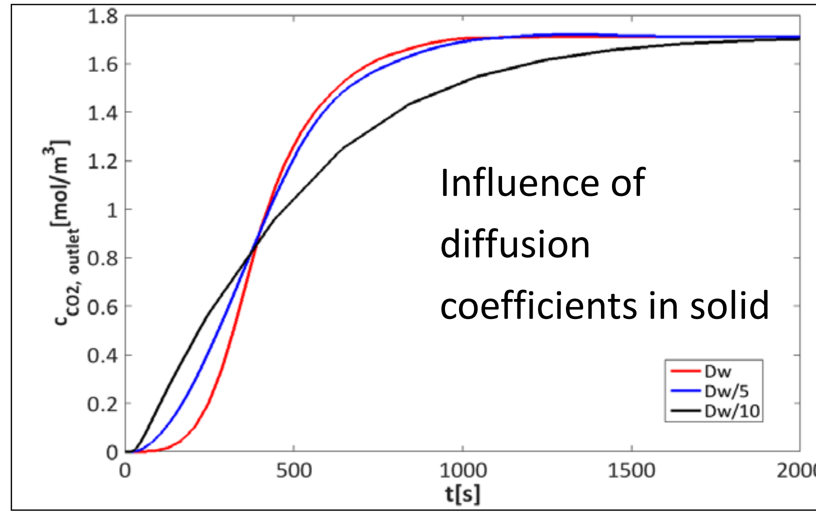


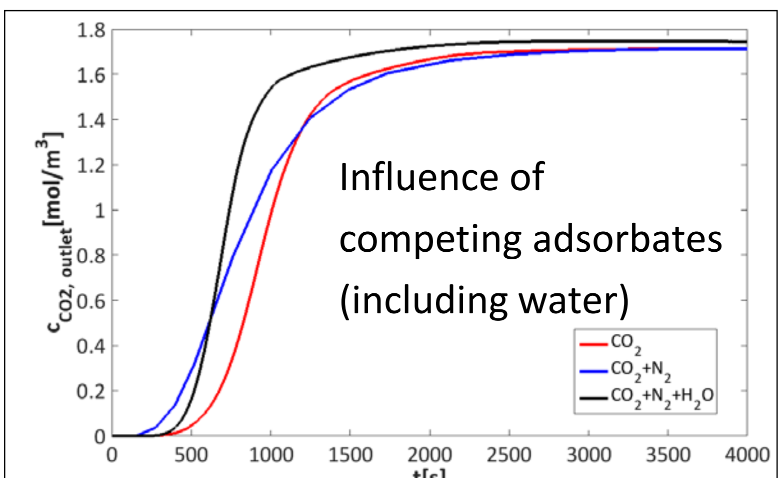
Solid temperature at certain position and time

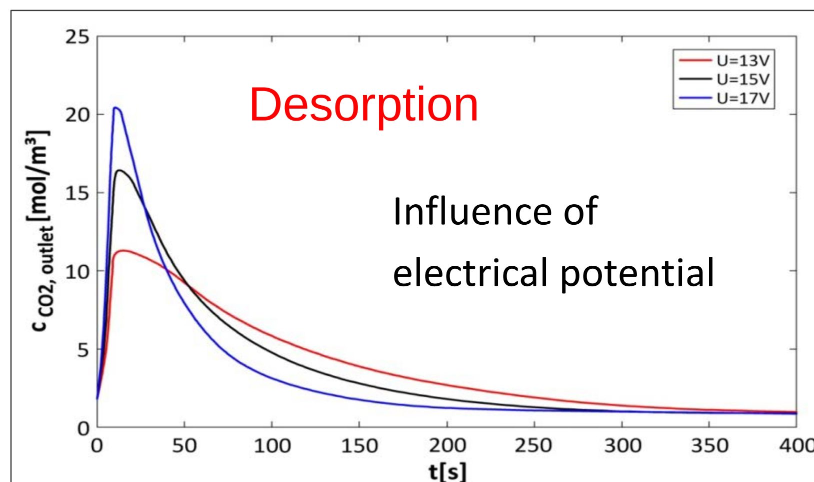
3D results – effect of parameters

CO_2 breakthrough curves









1D modelling

- Simplified model developed for the purpose of cycle design, simulations and analysis
- The model consists of non-stationary 1D material, energy and momentum balances for the gas phase (channel) and monolith wall mass and energy balance
- Implemented in gPROMS
- The 3D model simulation results used as “numerical experiments” for estimation of the 1D model parameters – model reduction study

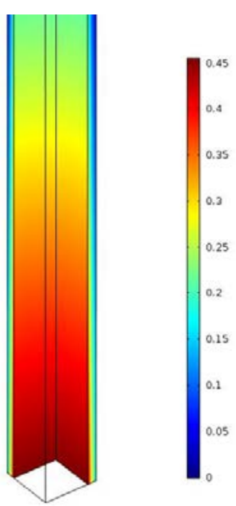
3D to 1D model reduction

$$\frac{\partial C_i}{\partial t} = \frac{1}{L_c^2}\frac{\partial}{\partial \varsigma}\left(D_{ax}\frac{\partial C_i}{\partial \varsigma}\right) - \frac{1}{L_c}\frac{\partial (C_i \upsilon_{ch})}{\partial \varsigma} - \rho_b \frac{\partial \bar{q}_i}{\partial t}\frac{(a_{ch}+2\Delta)^2 - a_{ch}^2}{a_{ch}^2}$$

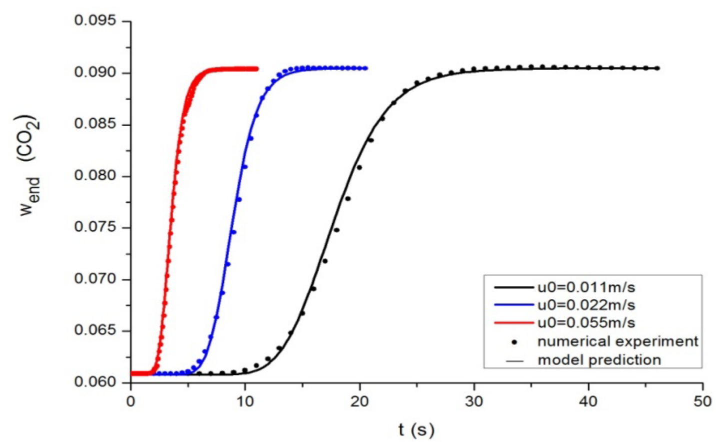
$$\frac{\partial \bar{q}}{\partial t} = k_i\left(q^* - \bar{q}\right)$$

$$\rho_g c_{p,g}\frac{\partial T_g}{\partial t} = \frac{1}{L_c^2}\frac{\partial}{\partial \varsigma}\left(D_{axh}\rho_g c_{p,g}\frac{\partial T_g}{\partial \varsigma}\right) - \frac{1}{L_c}\frac{\partial (T_g \upsilon_{ch}\rho_g c_{p,g})}{\partial \varsigma} - h\cdot(T_g - T_s)$$

$$\rho_b c_{p,s}\frac{\partial T_s}{\partial t} = \frac{1}{L_c^2}\frac{\partial}{\partial \varsigma}\left(\lambda_s\frac{\partial T_s}{\partial \varsigma}\right) + h\cdot(T_g - T_s)\frac{a_{ch}^2}{(a_{ch}+2\Delta)^2 - a_{ch}^2} + \rho_b\sum_{i=1}^{n}(-\Delta H_i)\frac{\partial \bar{q}_i}{\partial t} + \frac{U\cdot I_a}{\left((a_{ch}+2\Delta)^2 - a_{ch}^2\right)\cdot L_c}$$



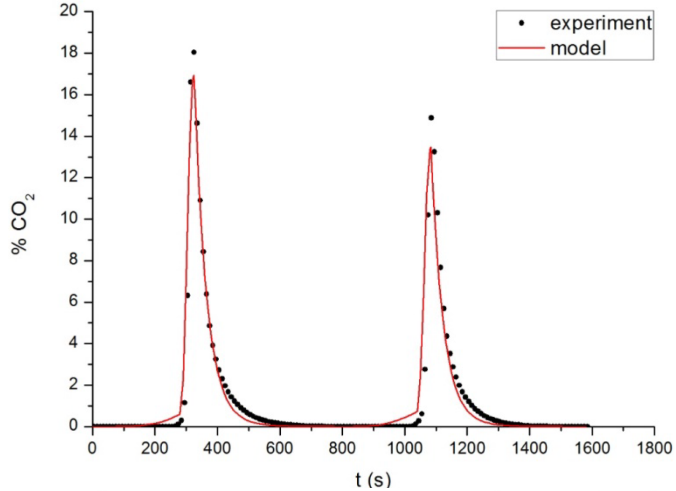
3D simulations under various conditions to estimate the key 1D model parameters – new correlations derived

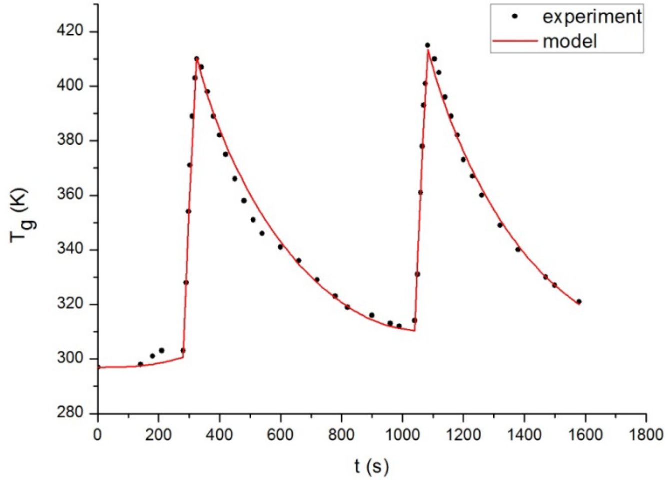


1D simulations and validation

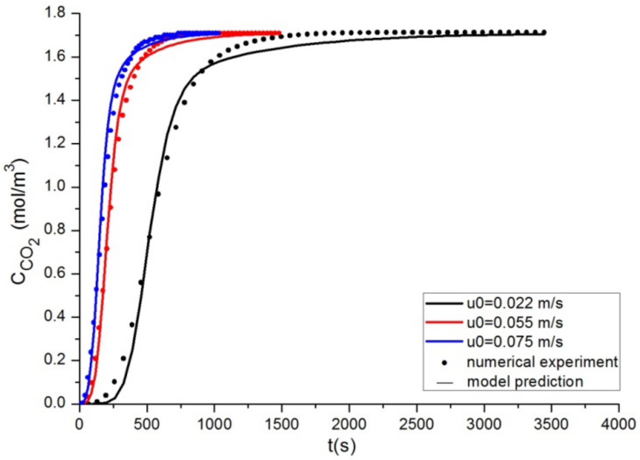
Validation based on

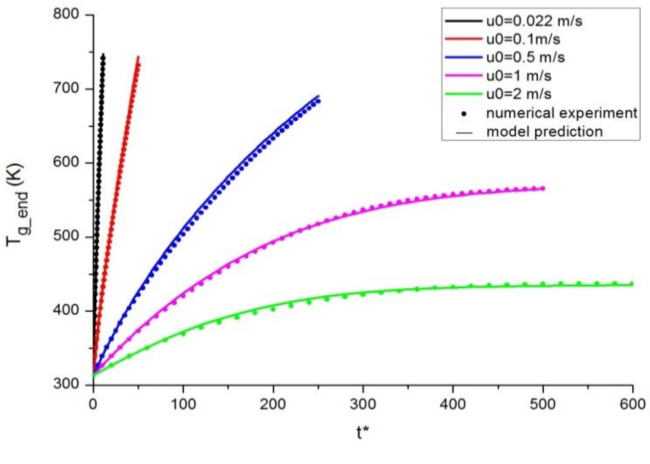
a) literature experimental data



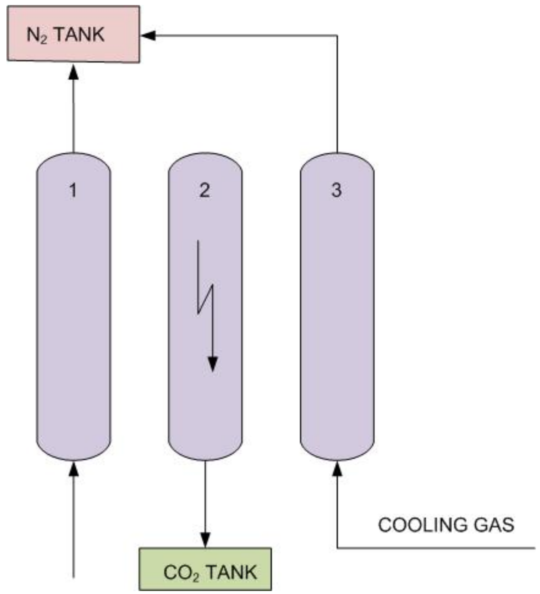


b) numerical 3D experiments





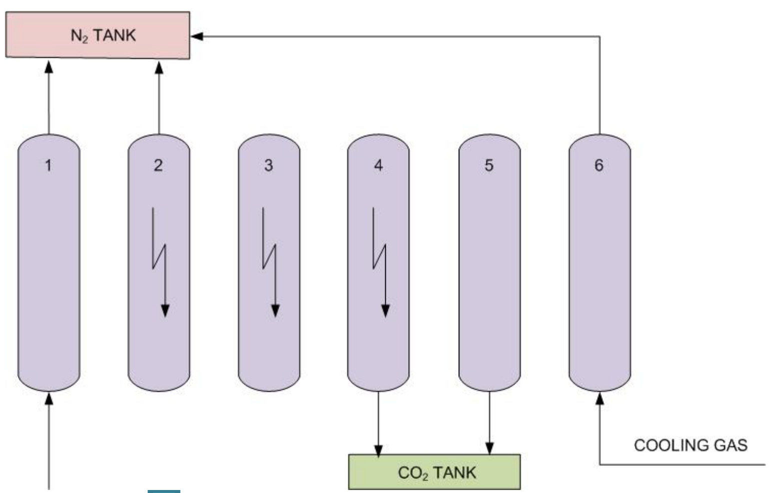
ESA cycle build-up



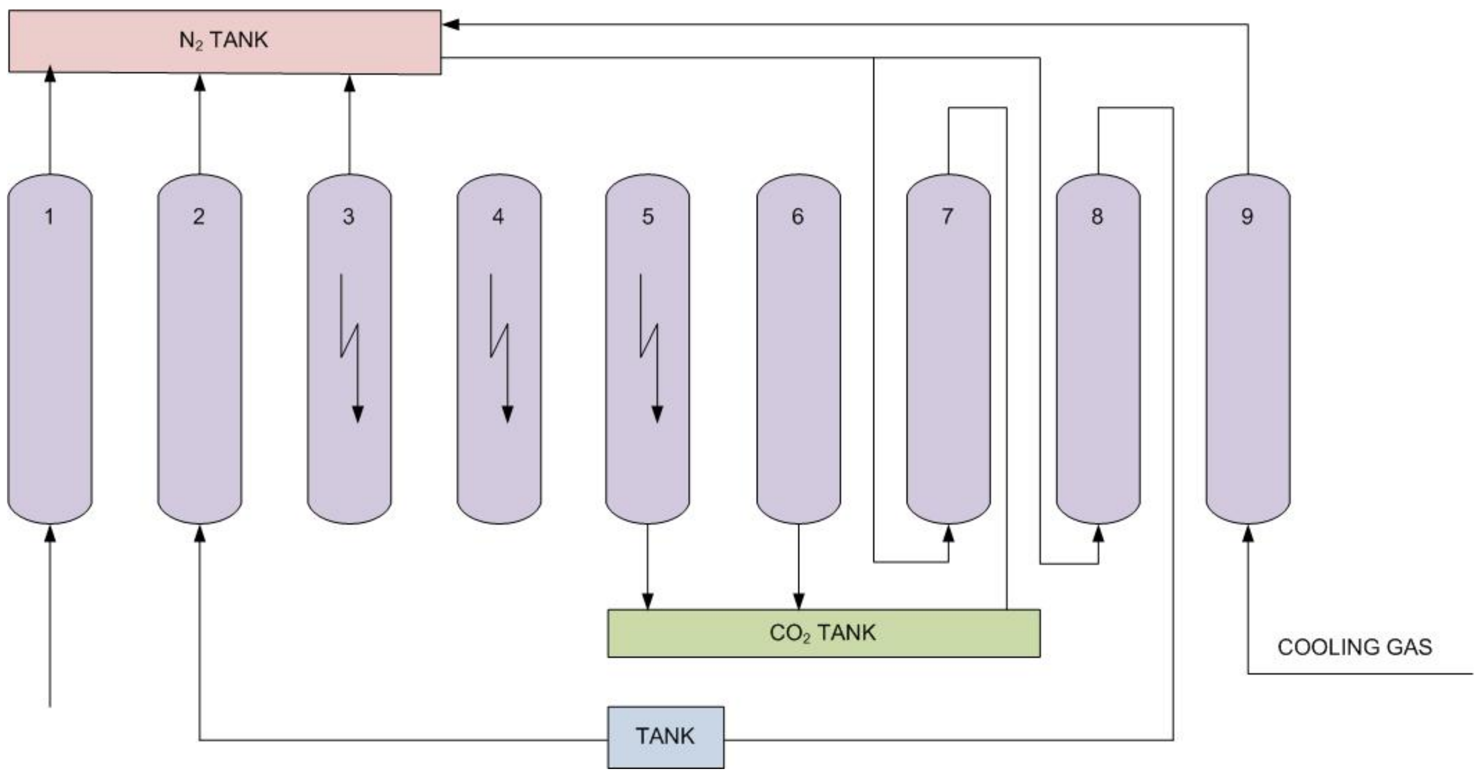
Simplest cycle with adsorption (**1**), desorption with electrification (**2**) and cooling (**3**) is far from satisfying P and R

Important: Water is removed in separate activated carbon adsorption columns and cycle

Adding rinse step (**2**), dividing electrification to 2 steps (**3** and **4**) and adding purge step (**5**) increased P to 91.5% and R to 79.2% - still not enough

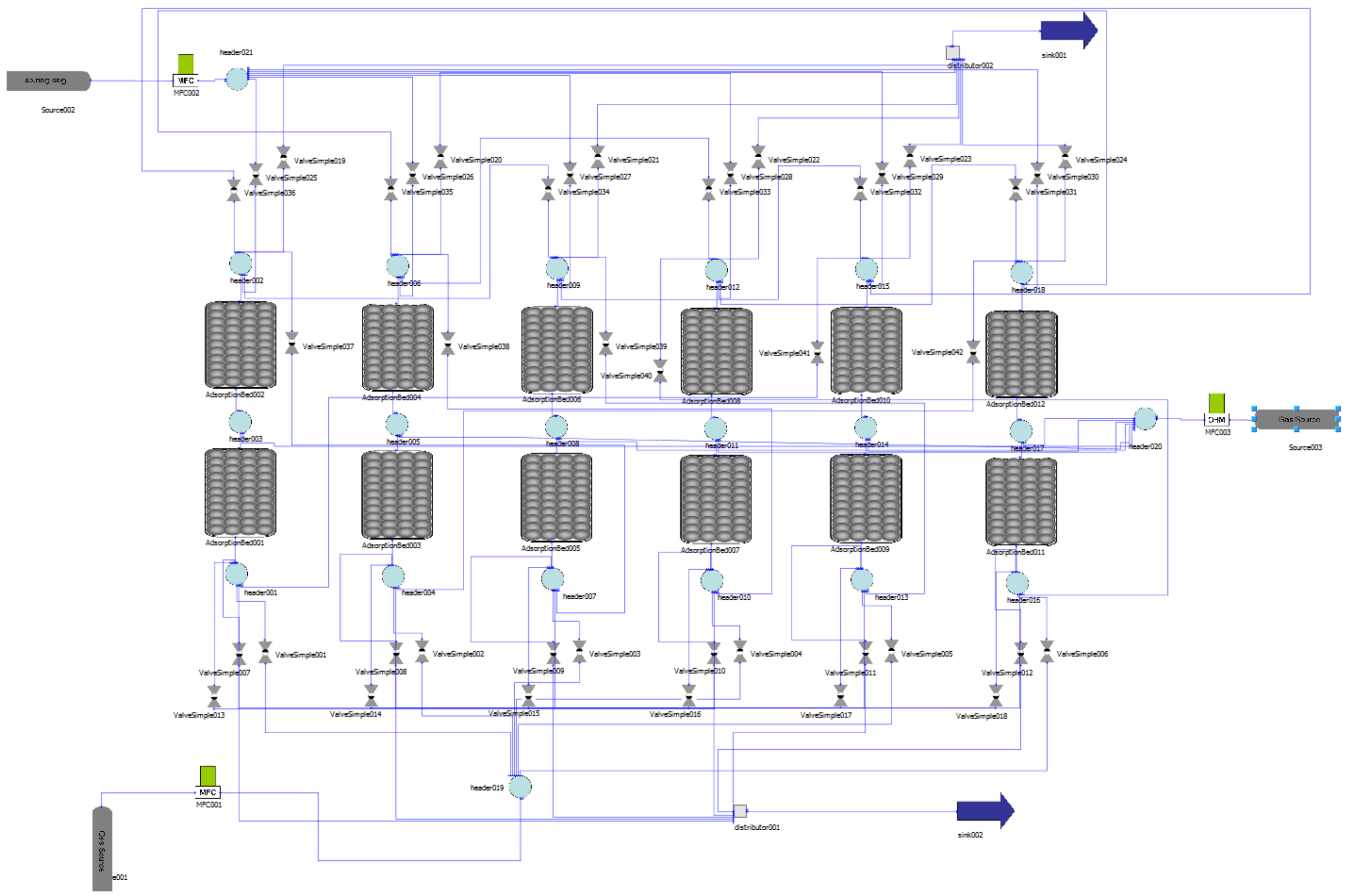


ESA cycle to reach P and R

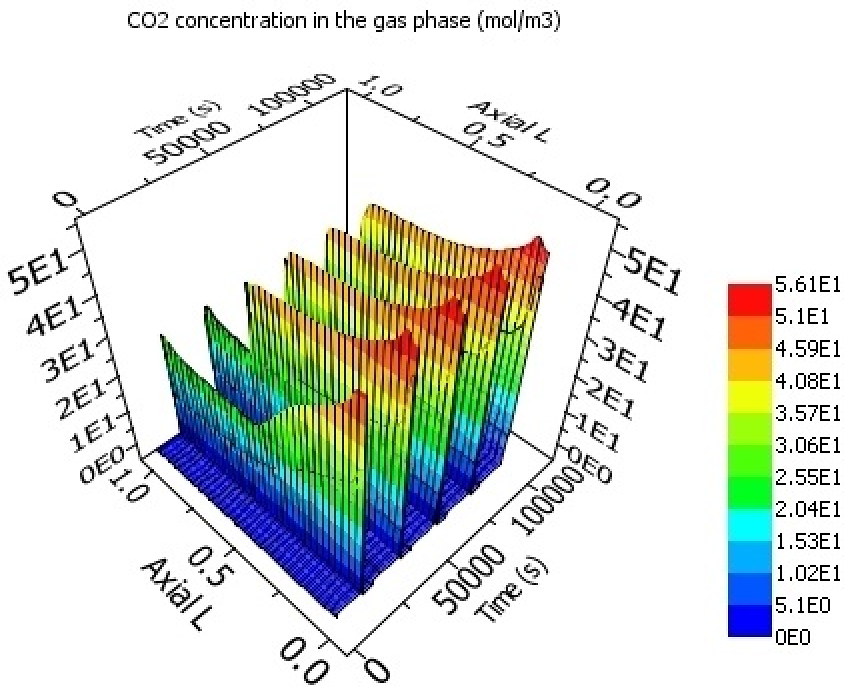


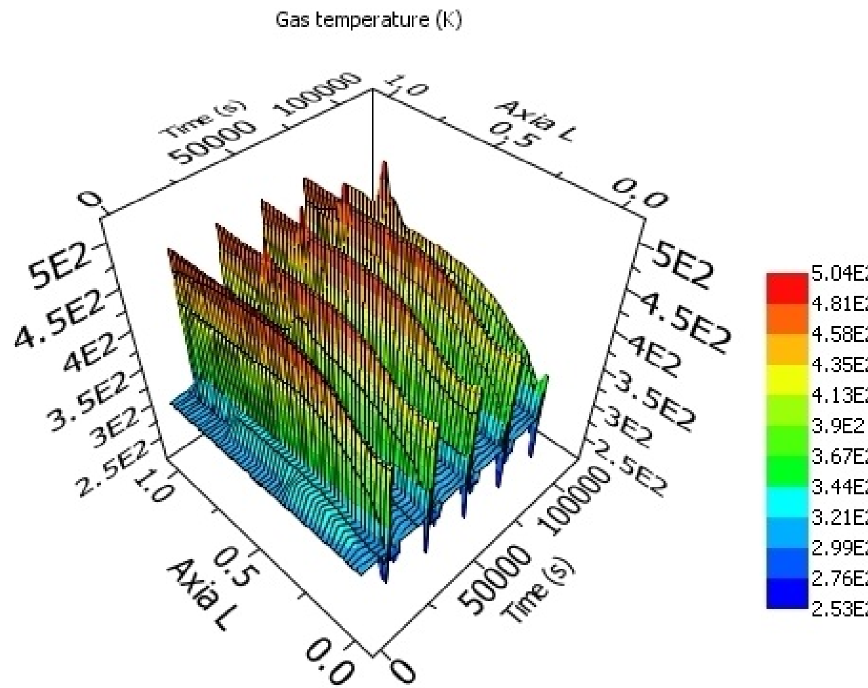
- Crucial step for reaching R is the recycle step, in which CO_2 that remained in the bed (new purge step – **8**) is returned to adsorb (before electrification – **2**)
- P is achieved by introduction of one more step during electrification (**5**)
- Cooling time is reduced as only 70% of the monolith is cooled to feed temp.

ESA cycle framework in gPROMS



ESA cycle results – long column (13X/carbon composite, 200 cpsi)





Purity = 95.40%

Recovery = 90.0%

Column legth **12m**

Total cycle time 5.61h

Adsorption: 3.87hr – **69**% of total time

Total regeneration: 1.74 h – **31**% of total time

Electrification: 0.28h – **5**% of total time

Cooling: 1.28 h – **23**% of total time

Results in numbers

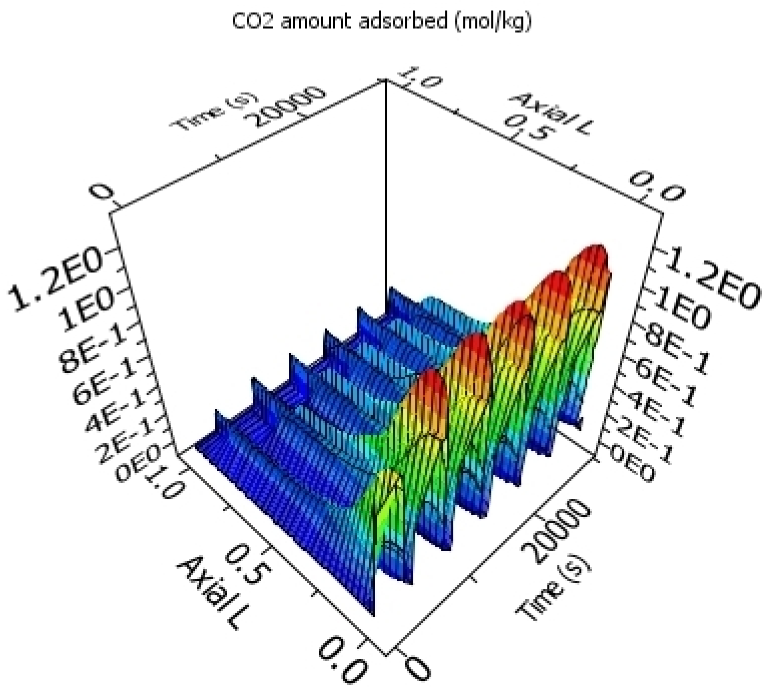
Total feed flow rate [Nm^3/s]	**480.7**
Inlet CO_2 fraction [%]	**3.5**
Maximal solid temperature [K]	**480**
CO_2 recovery rate [%]	**90.0**
CO_2 purity [%]	**95.4**
Mass of adsorbent in 1 column [t]	**348**
Total number of columns (12m long, 7.4m wide)	**60**
Total cycle time [h]	**5.61**
Adsorption time per total time [%]	**69**
Specific energy consumption [GJ/t_{CO2}]	**4.41**

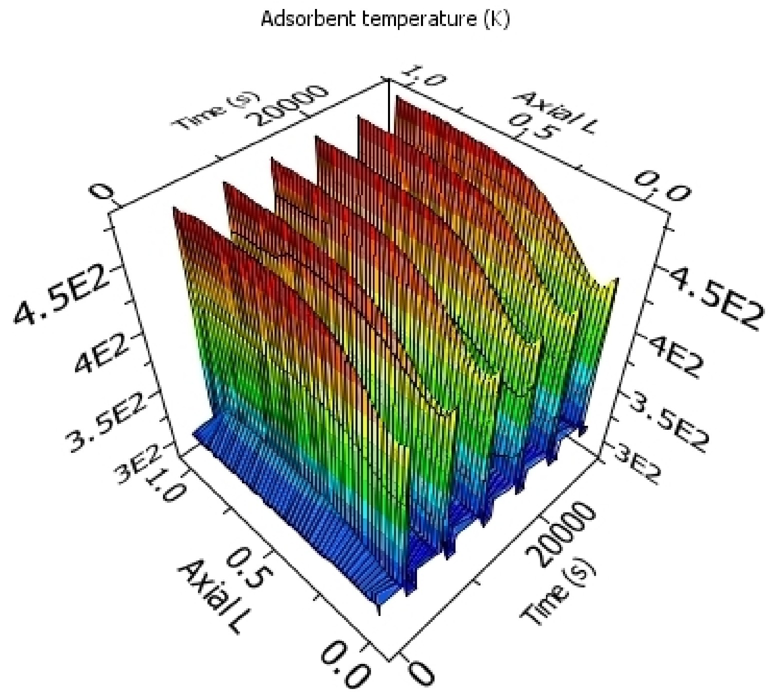
Energy cost for reaching R and P

- If **R** and P are lower electric energy consumption decreases considerably:

Space-average T during desorption [K]	Purity [%]	Recovery [%]	Specific energy consumption [GJ/t_{CO2}]
435	95.1	79.3	3.58
445	96.3	83.6	3.85
455.5	95.2	87.2	4.08
465	95.5	89.1	4.33
468.1	95.4	90.0	4.41

ESA cycle results – short column





Purity =96.3 %

Recovery =87.5 %

Column length 2.9 **m**

Cycle time 1.43 h

Adsorption: 0.89 hr – 62 % of total time

Total regeneration: 0.54 hr –38 % of total time

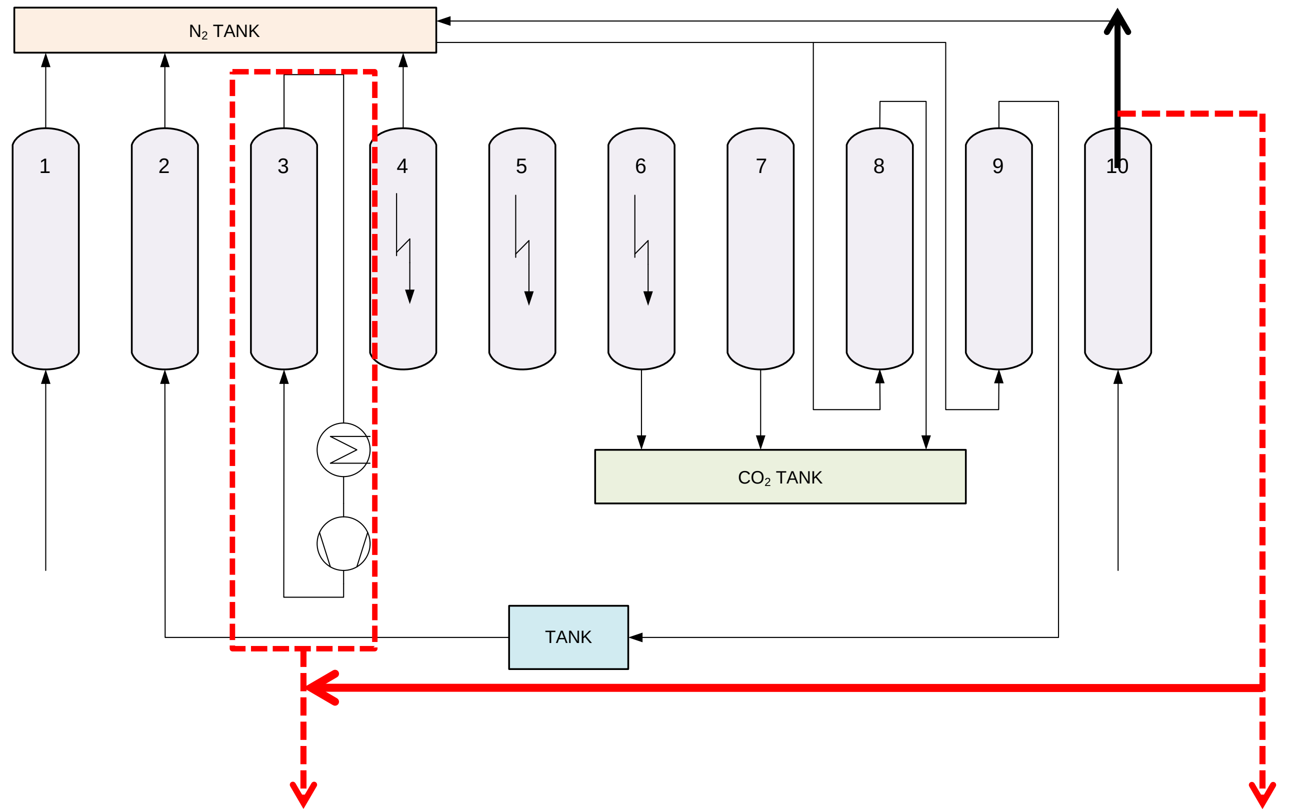
Electrification: 0.15 hr – 10.5 % of total time

Cooling: 0.33 hr –23 % of total time

Results in numbers

Total feed flow rate [Nm^3/s]	**480.7**
Inlet CO_2 fraction [%]	**3.5**
Maximal solid temperature [K]	**480**
CO_2 recovery rate [%]	**87.5**
CO_2 purity [%]	**96.2**
Mass of adsorbent per column [t]	**86.94**
Total number of columns (3m long, 7.4m wide)	**60**
Total cycle time [h]	**1.43**
Adsorption time per total time [%]	**62**
Specific energy consumption [GJ/t_{CO2}]	**4.62**

ESA cycle – heat integration



- Heat integration within the cycle and with the water removal unit
- Heat integration with low-grade steam from the power-plant
- The specific energy consumption expected to drop to **2.5 GJ/t_{CO2}**

Summary

- Within MATESA project, models for ESA process, suitable for complex cycle simulations and optimisation, have been developed and exploited
- The ESA cycle simulations show that the requirements of high purity (>95%) and recovery (>90%) can be achieved, though through complex cycle design with a number of steps and recycles
- The results indicate that the ESA process based on zeolite or MOF-carbon composite monoliths can be an alternative to absorption based processes for CO_2 capture
- Further impovements trough further material development and optimisation and energy integration are foreseen