



## Measurement of properties and pilot testing. CERE lab and model development

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# Measurement of properties and pilot testing

CERE lab and model development

Application: Rate based modeling of CO<sub>2</sub> capture

**Philip Loldrup Fosbøl**  
 + many students and faculty

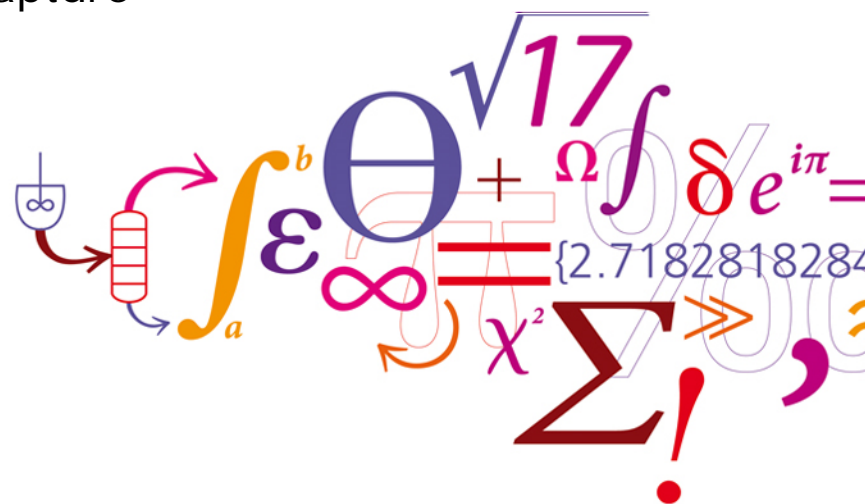
EFCE WP, May 12<sup>th</sup> 2016

**CERE**

Center for Energy Resources Engineering

**DTU Chemical Engineering**

Department of Chemical and Biochemical Engineering

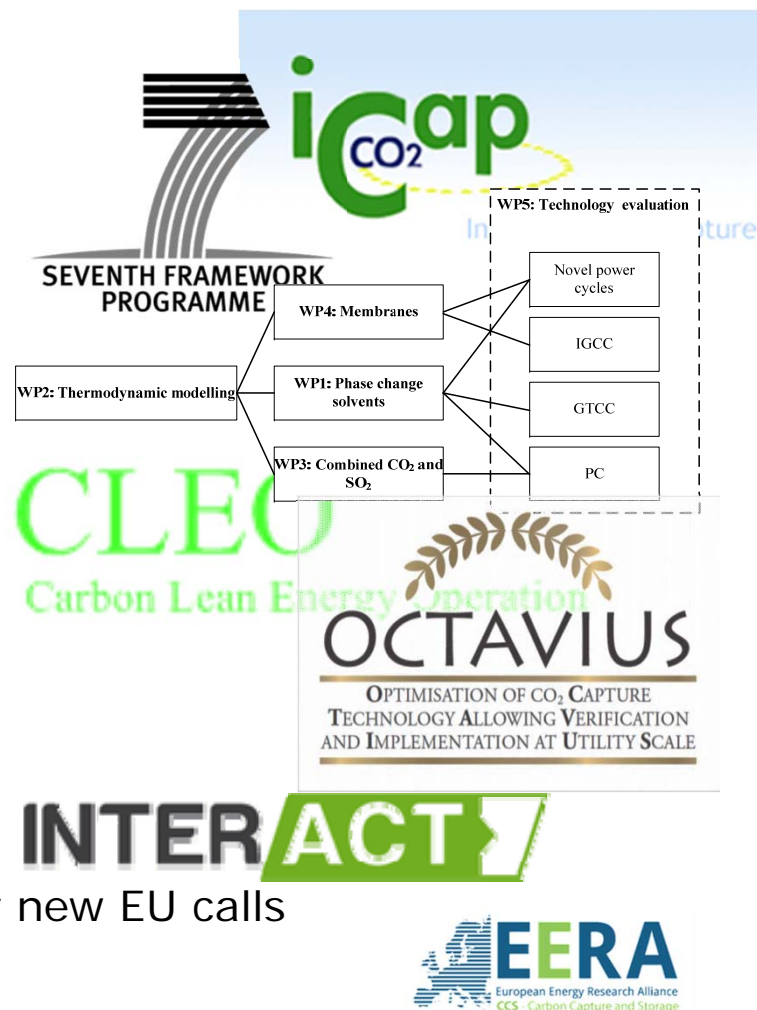


# CERE Industrial Consortium 2016

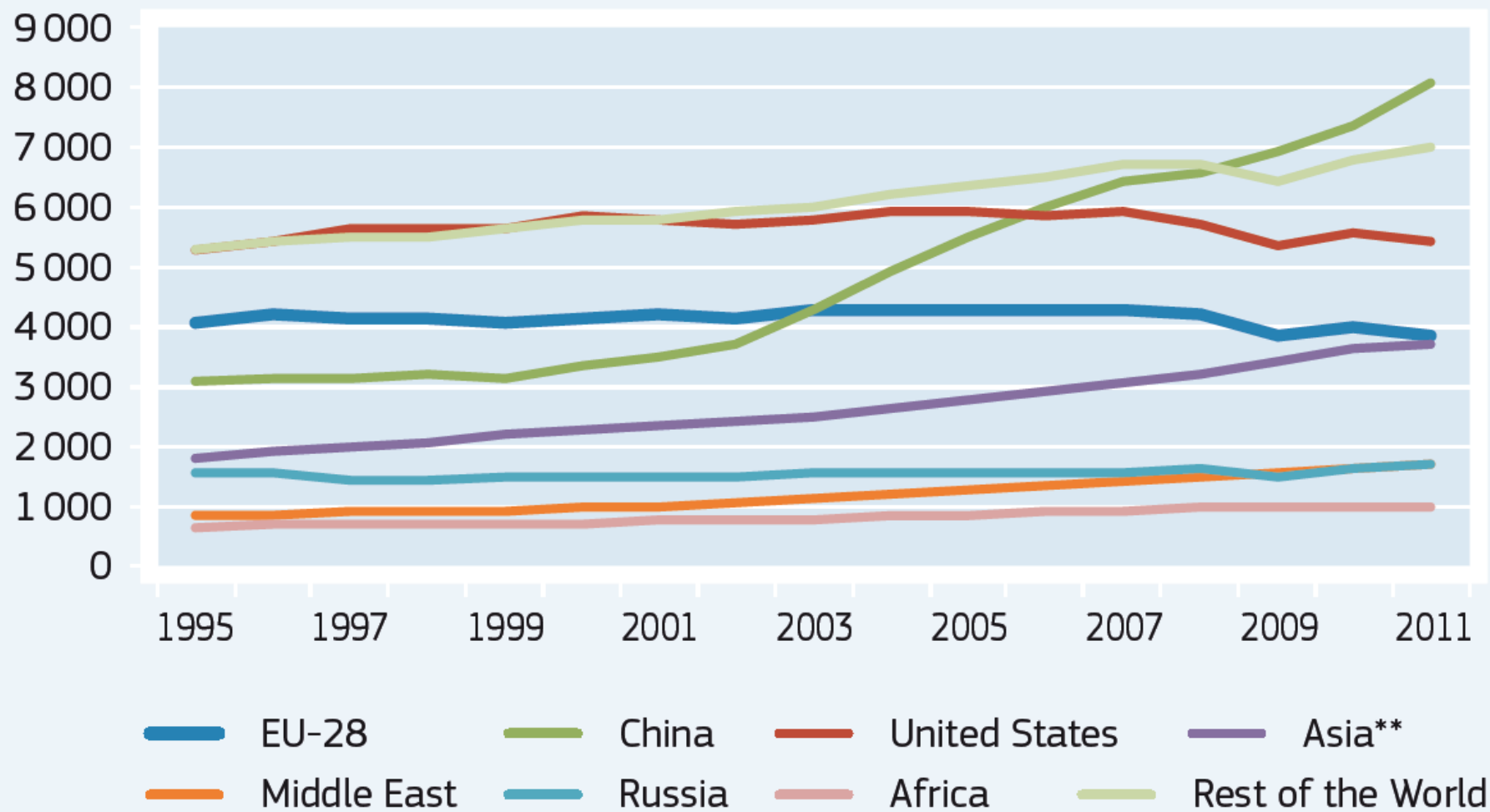


## EU Activities

- CASTOR
  - FP6 EU project
- iCap
  - Gas hydrate
  - Demixing process
- CESAR/CLEO
  - Thermodynamic model implementation
  - CASTOR comparison
- OCTAVIUS
  - Process Benchmarking
  - CAPE-Open development
- INTERACT
  - Lab scale & pilot trials using enzymes
- EERA
  - Preparation of consortia idea creation for new EU calls



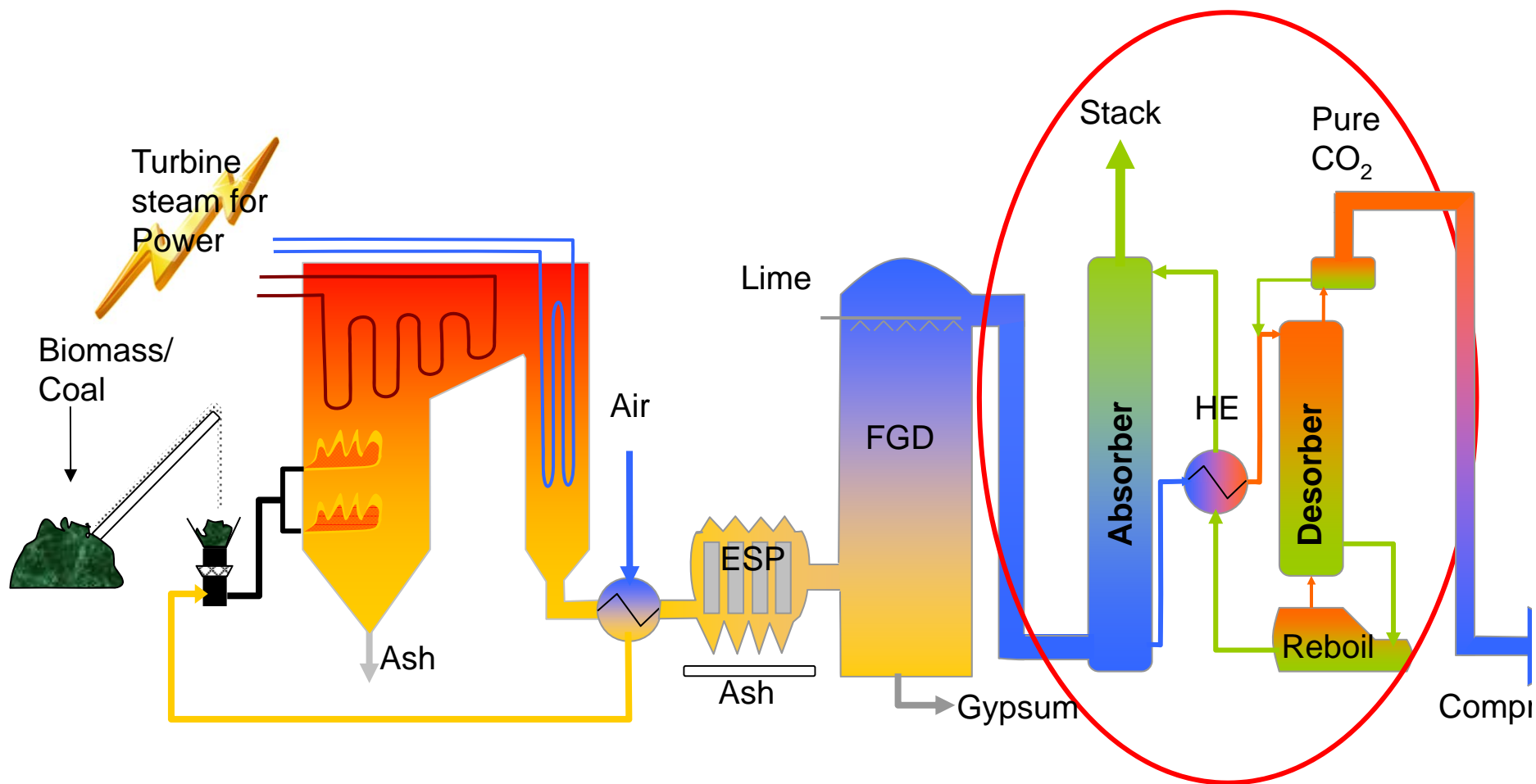
## World CO<sub>2</sub> Emissions by Region (Mio ton CO<sub>2</sub>)



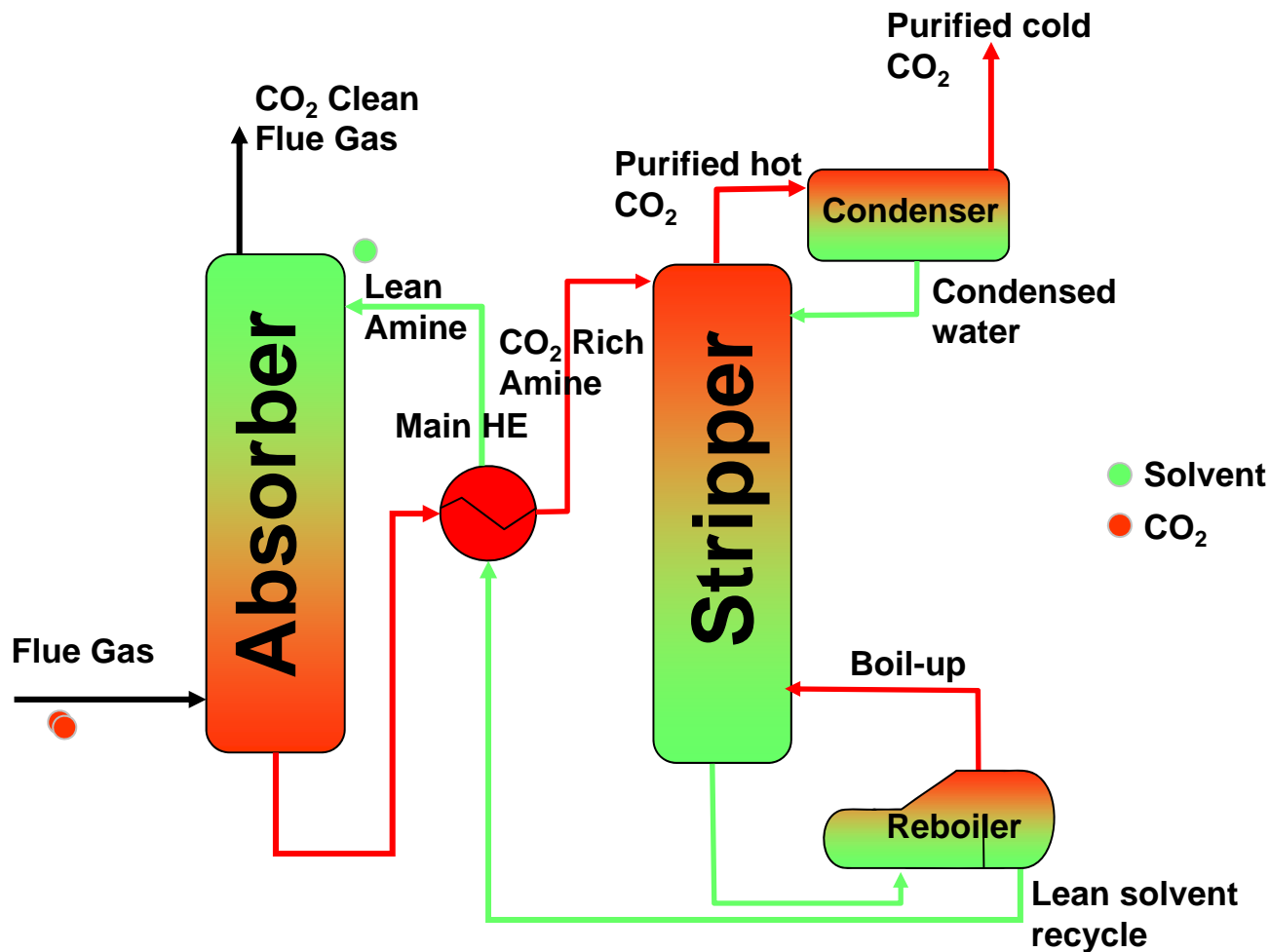
EU energy in figures 2014

# Australian “Coal Mountain”

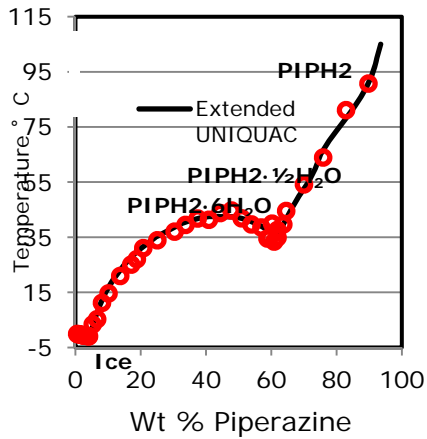
# Carbon capture and storage (CCS)



# CO<sub>2</sub> capture





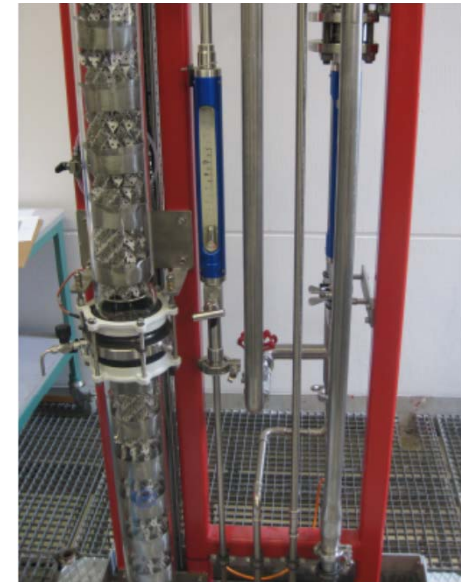


### Modelling

- Energy consumption
- Heat of reaction
- Thermodynamics
- Kinetics

### Pilot tests

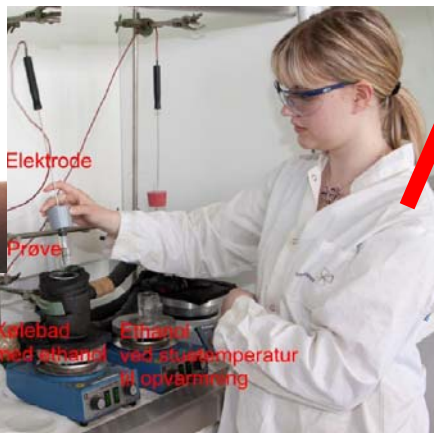
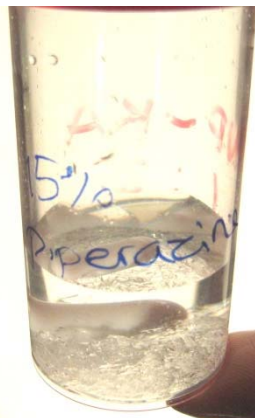
- Real life tests
- Solvent study
- Packing testing
- Energy requirements
- Mass transfer



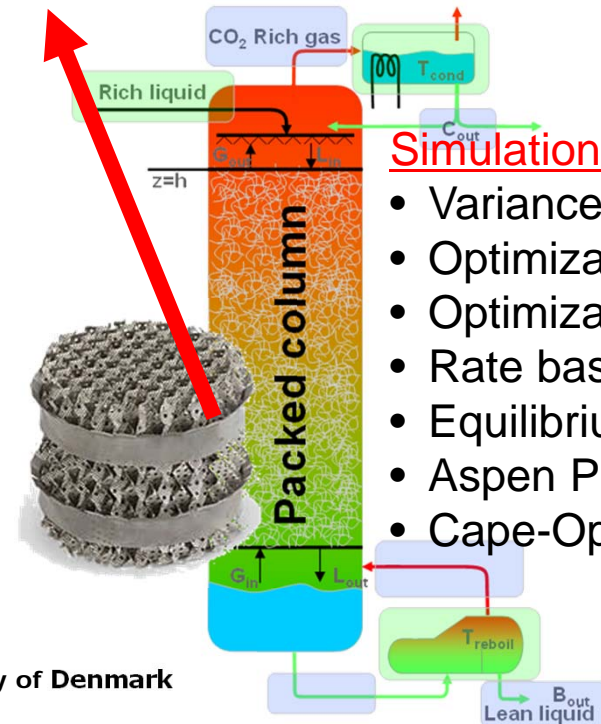
# Emission **CO<sub>2</sub>** reduction

### Experimental

- Physical Properties
- Equilibrium
- Kinetics



Karlebæd med alkalisk Elektrode ved stuetemperatur til opvarmning



### Simulation

- Variance analysis
- Optimization of energy use
- Optimization of packing
- Rate based approach
- Equilibrium approach
- Aspen Plus
- Cape-Open

# Rate based model (CapCO<sub>2</sub>)

- Gas balance

Total: 
$$\frac{dG}{dz} = -(N_C + N_W) aS$$

CO<sub>2</sub>: 
$$G \frac{dy_C}{dz} = -y_C \frac{dG}{dz} - N_C aS$$

H<sub>2</sub>O: 
$$G \frac{dy_W}{dz} = -y_W \frac{dG}{dz} - N_W aS$$

Energy: 
$$G C_{p,tot}^G \frac{dT_G}{dz} = - \left( \frac{dG}{dz} C_{p,tot}^G + aS (C_{p,W}^G N_W + C_{p,C}^G N_C) \right) T_G - qaS$$

- Liquid balance

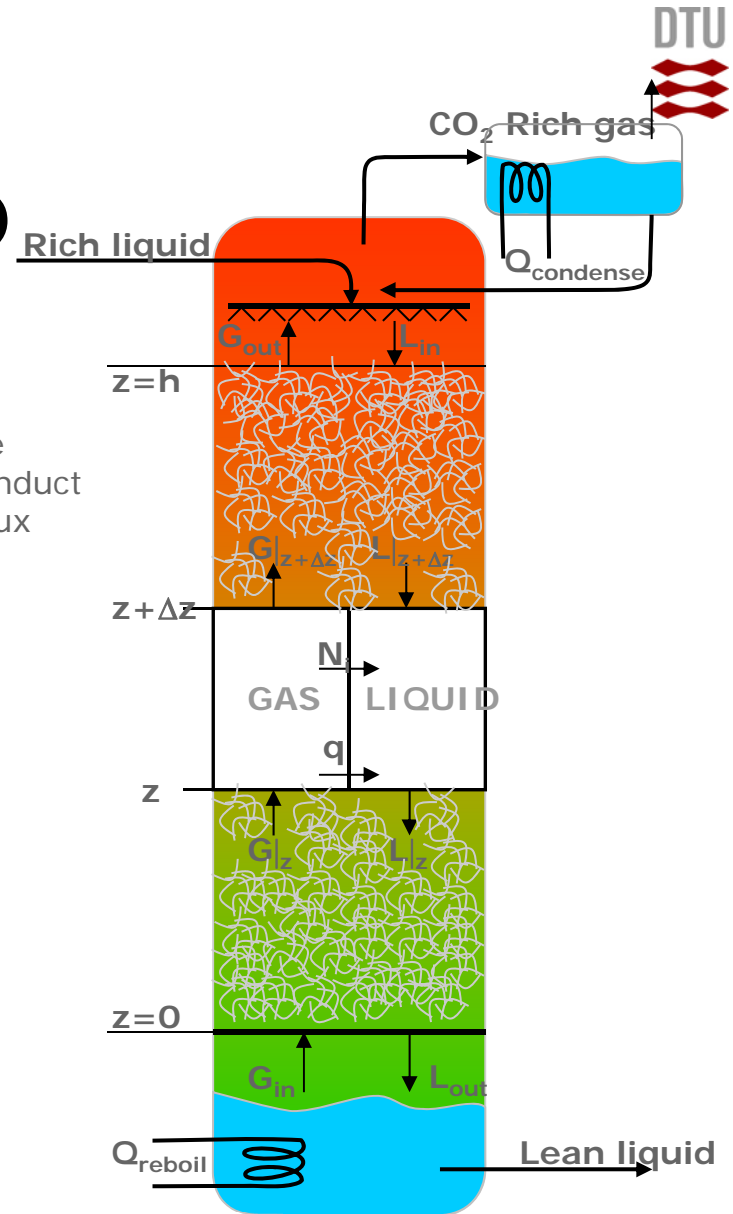
Total: 
$$\frac{dL}{dz} = -N_W aS$$

CO<sub>2</sub>: 
$$L \frac{dx_C}{dz} = -x_C \frac{dL}{dz} - N_C aS$$

H<sub>2</sub>O: 
$$L \frac{dx_W}{dz} = -x_W \frac{dL}{dz} - N_W aS + N_C aS$$

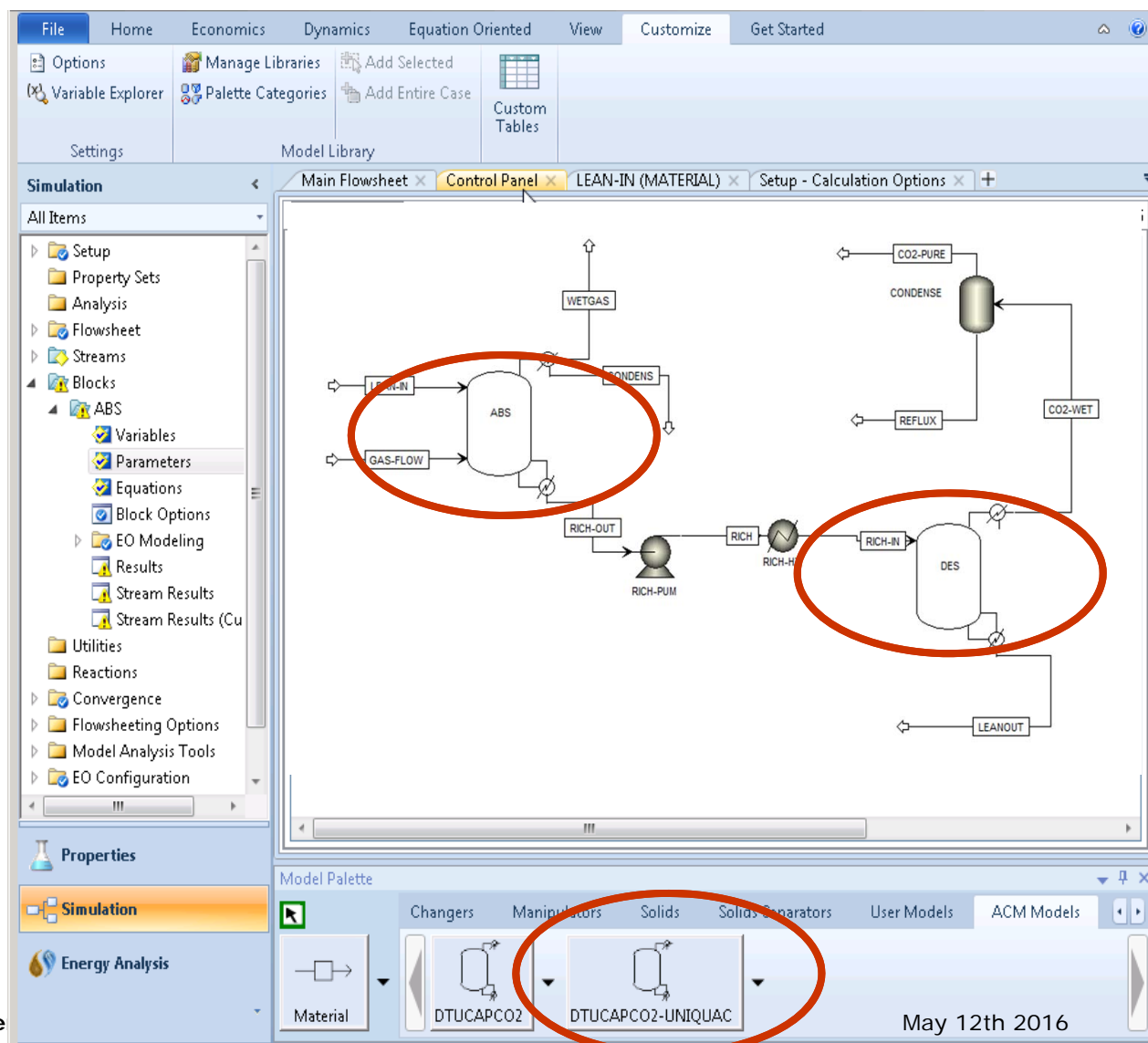
Energy: 
$$C_{p,tot}^L L \frac{dT_L}{dz} = -C_{p,tot}^L T_L \frac{dL}{dz} - aS \left( (C_{p,W}^L T_G + \Delta_{vap} H_W(T_L)) N_W + (C_{p,C}^L T_G + \Delta_{CO_2,diss} H(T_L)) N_C \right) - qaS$$

W: H<sub>2</sub>O  
 C: CO<sub>2</sub>  
 G: Gas  
 L: Liquid  
 z: Distance  
 q: Heat conduct  
 N: Mass Flux



# CAPCO<sub>2</sub> unit operation

Aspen  
Plus



# Physical properties in Rate based modelling

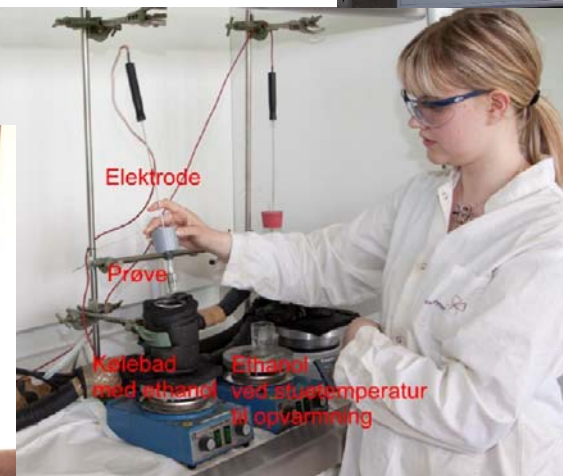
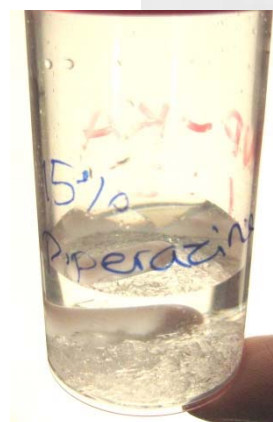
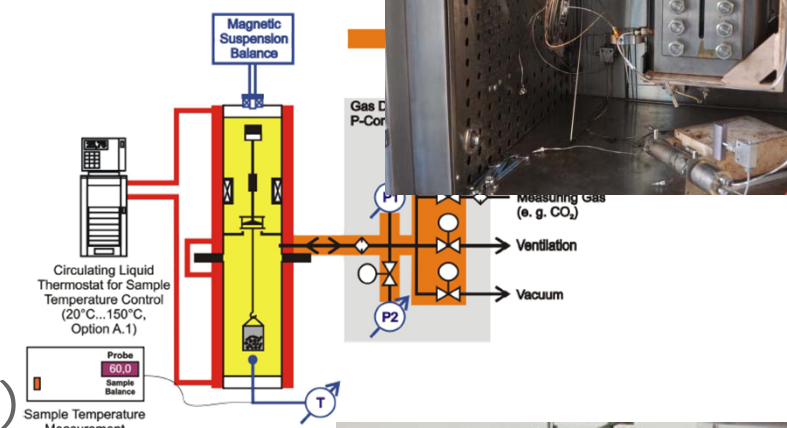
- **Liquid** properties
  - Diff. coef. A in W
  - Diff. coef. CO<sub>2</sub> in A-W sol.
  - Surface tension of W and A-W sol.
  - Viscosity of A-W sol.
  - Second order **rate constant** of CO<sub>2</sub> abs. in A-W
  - Thermodynamic properties
    - Heat cap. of solution
    - Henry's constant of CO<sub>2</sub> in A-W sol.
    - Equilibrium CO<sub>2</sub> pressure over A-W sol.
    - Heat of abs. of CO<sub>2</sub> in A-W sol.
    - Saturation pressure of W
    - Heat of vaporization of W
    - Density of pure W, A, and sol.
  
- **Gas** properties
  - Diffusivity of CO<sub>2</sub> in gas
  - Diffusivity of W in gas
  - Viscosity of gas (CO<sub>2</sub>-Air-W)
  - Thermodynamic properties
    - Density of gas
    - Heat cap. of gas (CO<sub>2</sub>, Air, W)

W: Water  
 A: Amine  
 Sol.: Mixture

# Phase eq. & properties

- CO<sub>2</sub> solubility
  - VLE
  - High P and T
- Slurry formation(SLE)
  - Freezing point depression
  - Solubility measurement
- Density
- Viscosity
- Surface tension

MSB equipped with gas pressure generation and control

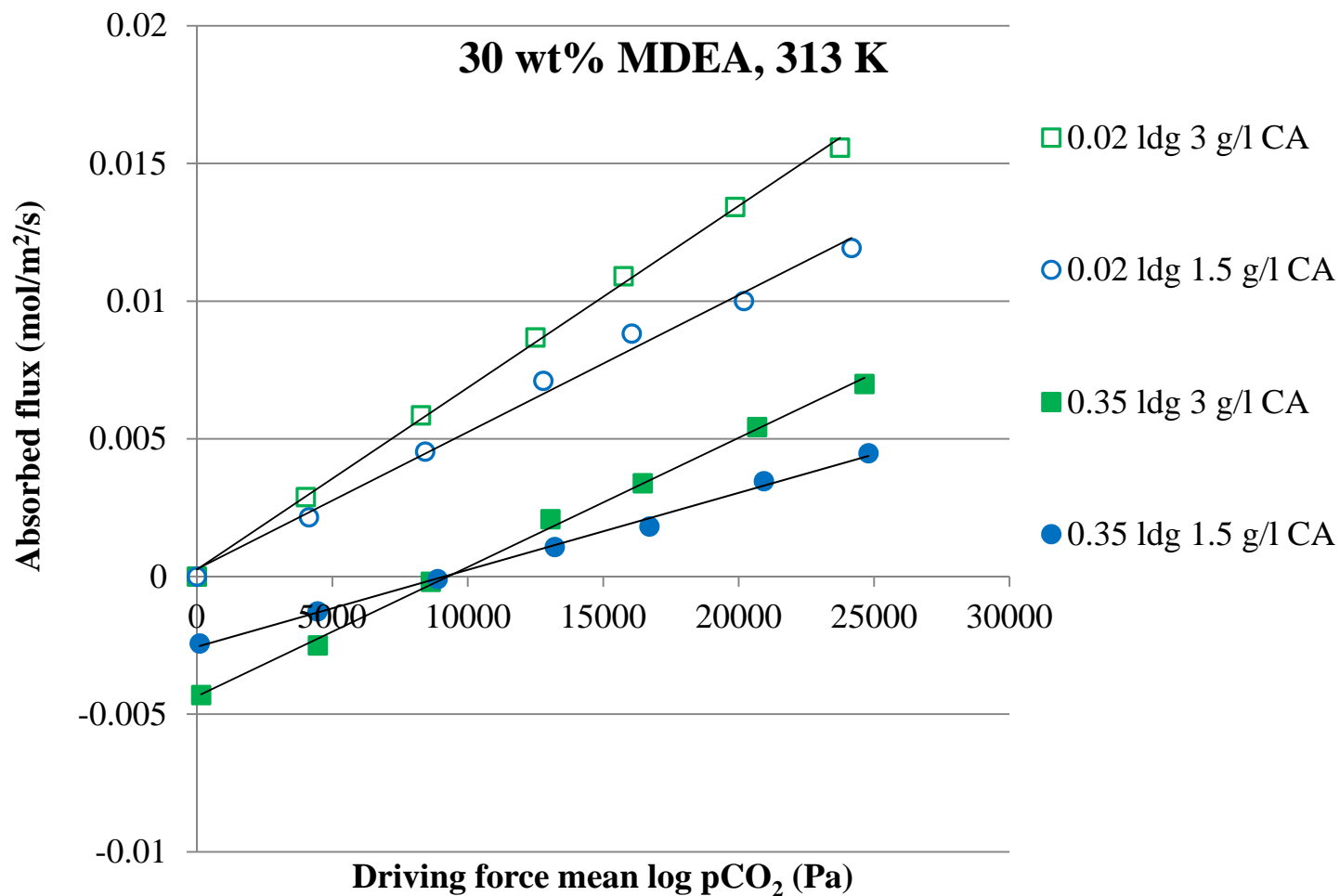




# Reaction kinetics between CO<sub>2</sub> and solvent

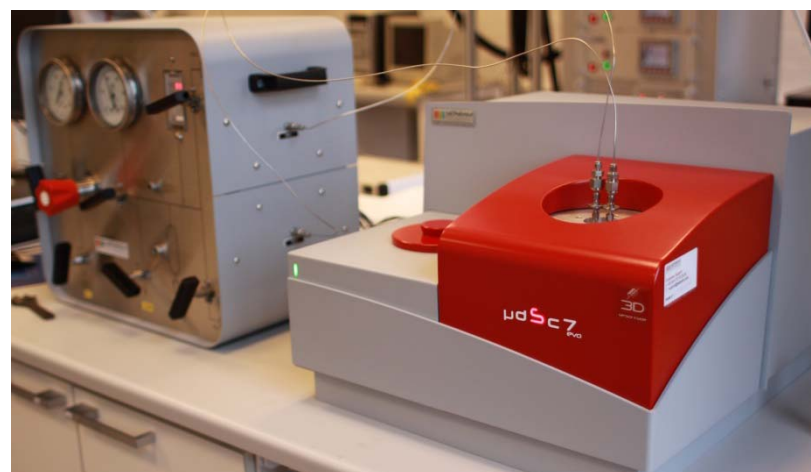


# Kinetic result



## Experimental work - calorimetric

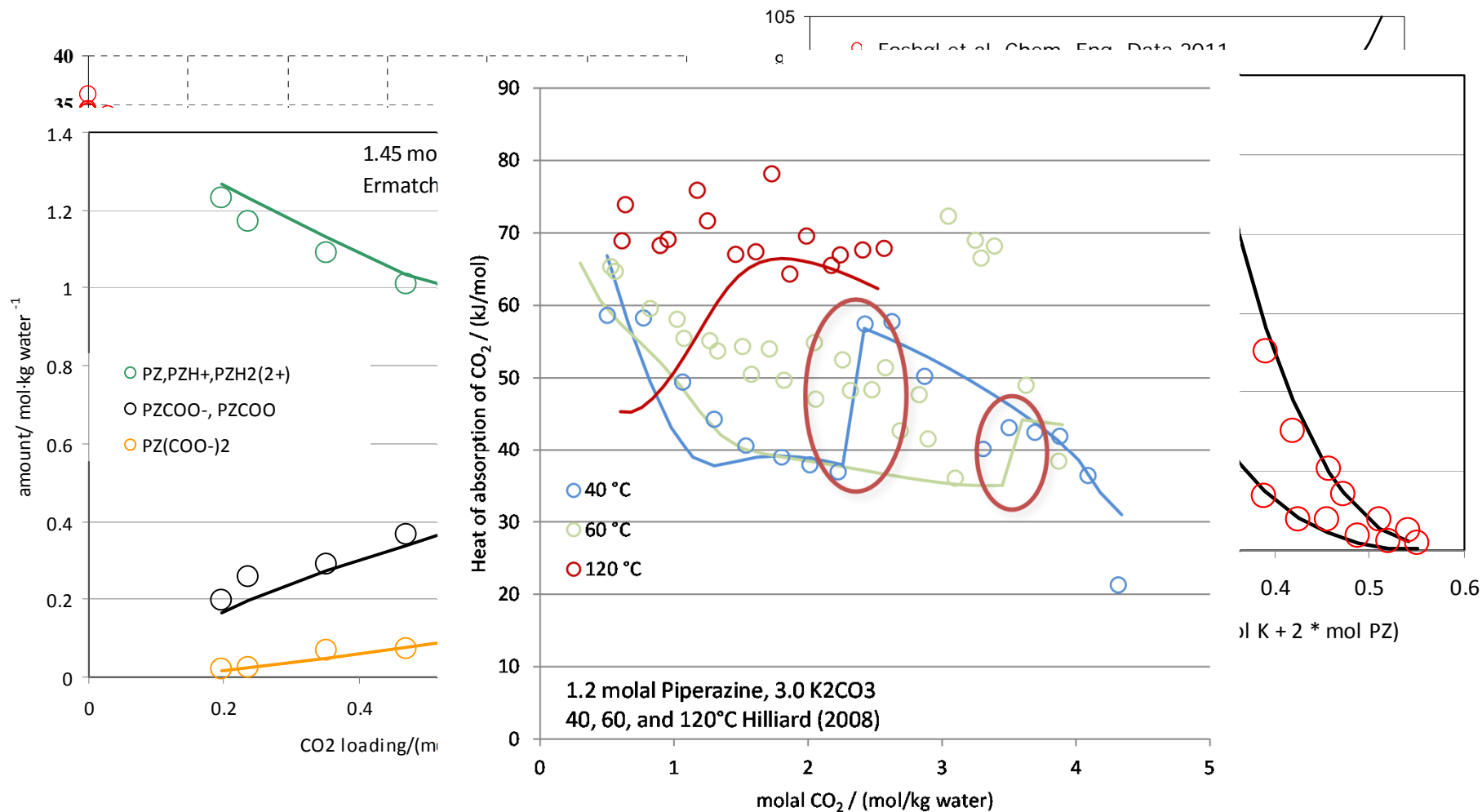
- High pressure DSC
- Phase change, heat of absorption by DSC





# Thermodynamic modelling

## ex: $\text{CO}_2\text{-PZ-K}_2\text{CO}_3\text{-KHCO}_2\text{-H}_2\text{O}$



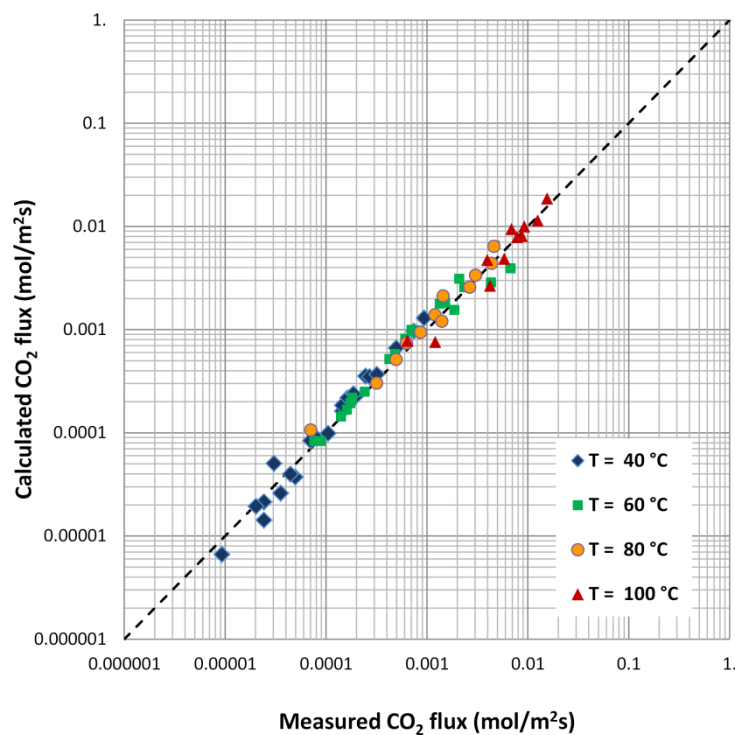
## Pilot tests and demonstration

- CO<sub>2</sub> Absorber
  - 10m height (Variable height)
  - 10cm diameter
  - Capacity: Approximately 40Nm<sup>3</sup>/h
  - Structured packing (Mellapack)
  - Temperature and sampling readings
    - Every meter
    - Temperature and loading profiles
  - Well developed DAQ for flow etc.
- Absorber test runs
  - Standard Amines
  - Enzymes
- Desorber
  - Design in progress

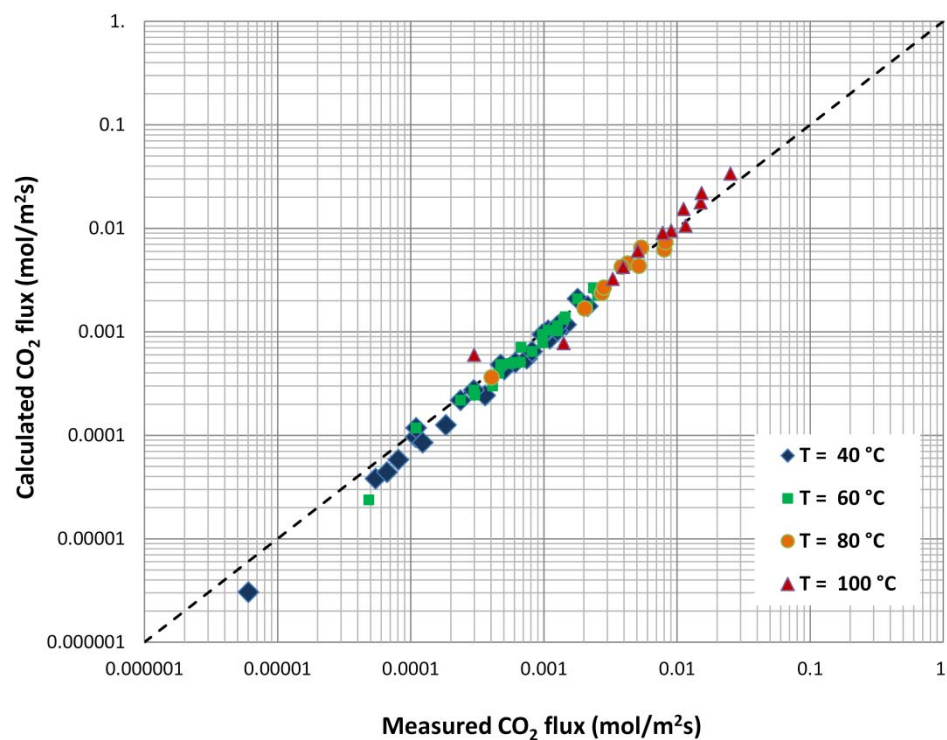


# Mass Transfer Modeling

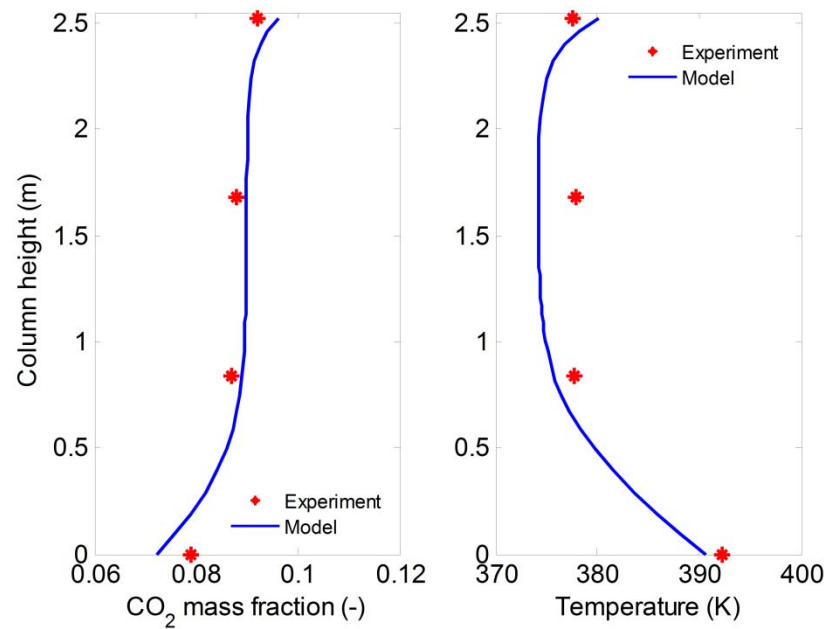
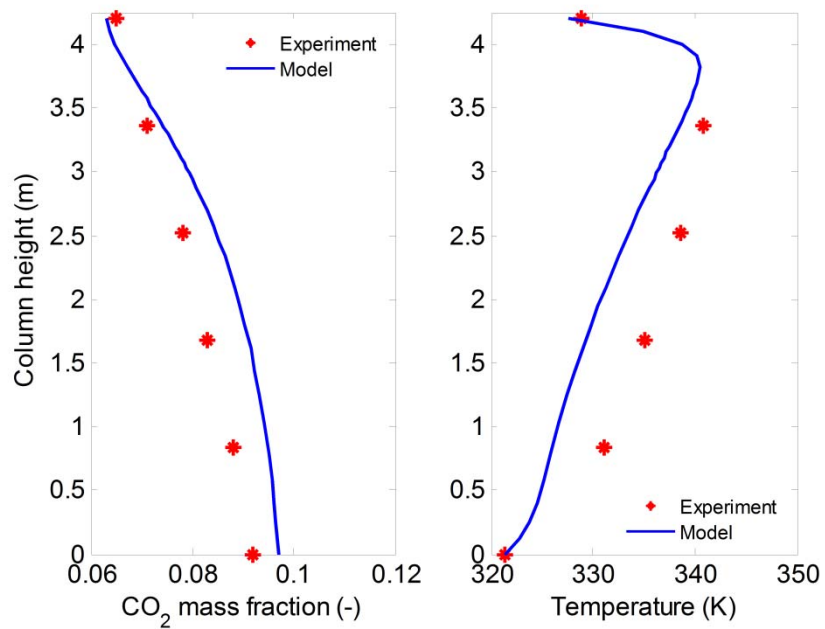
30 wt.% MEA



5 molal PZ



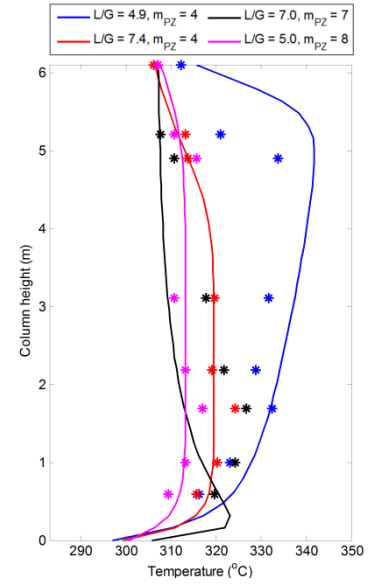
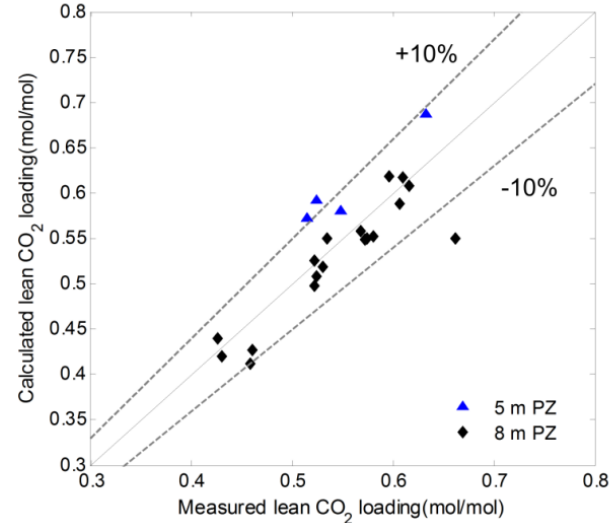
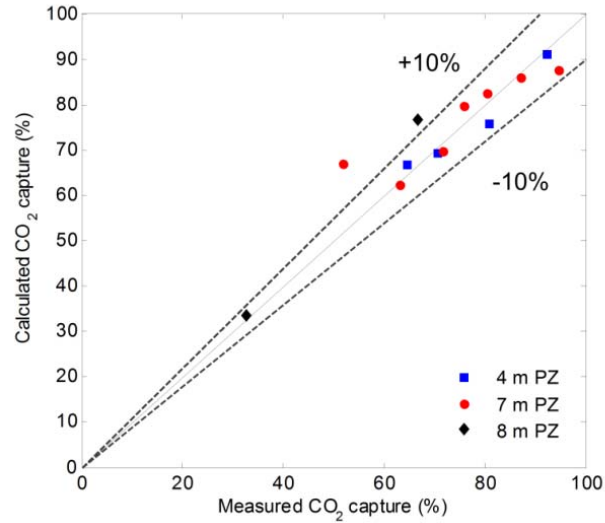
# Comparison to pilot data



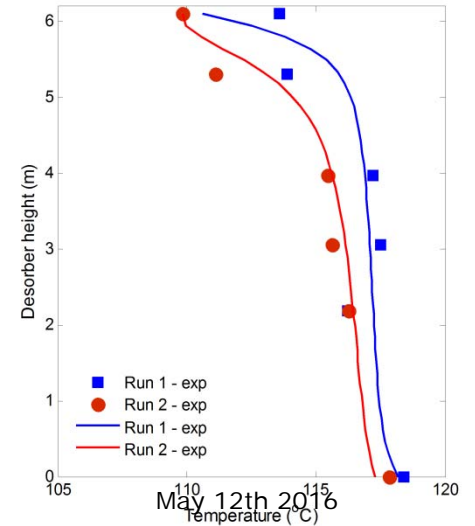
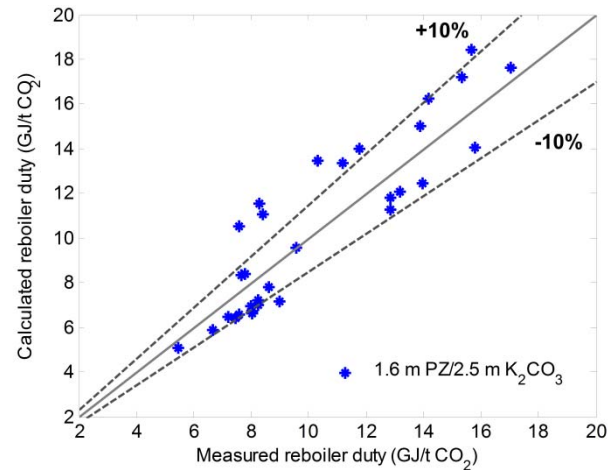
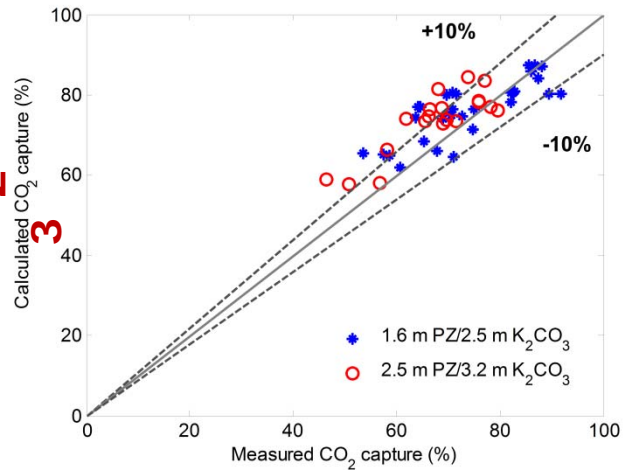
# Modeling Innovative Solvents



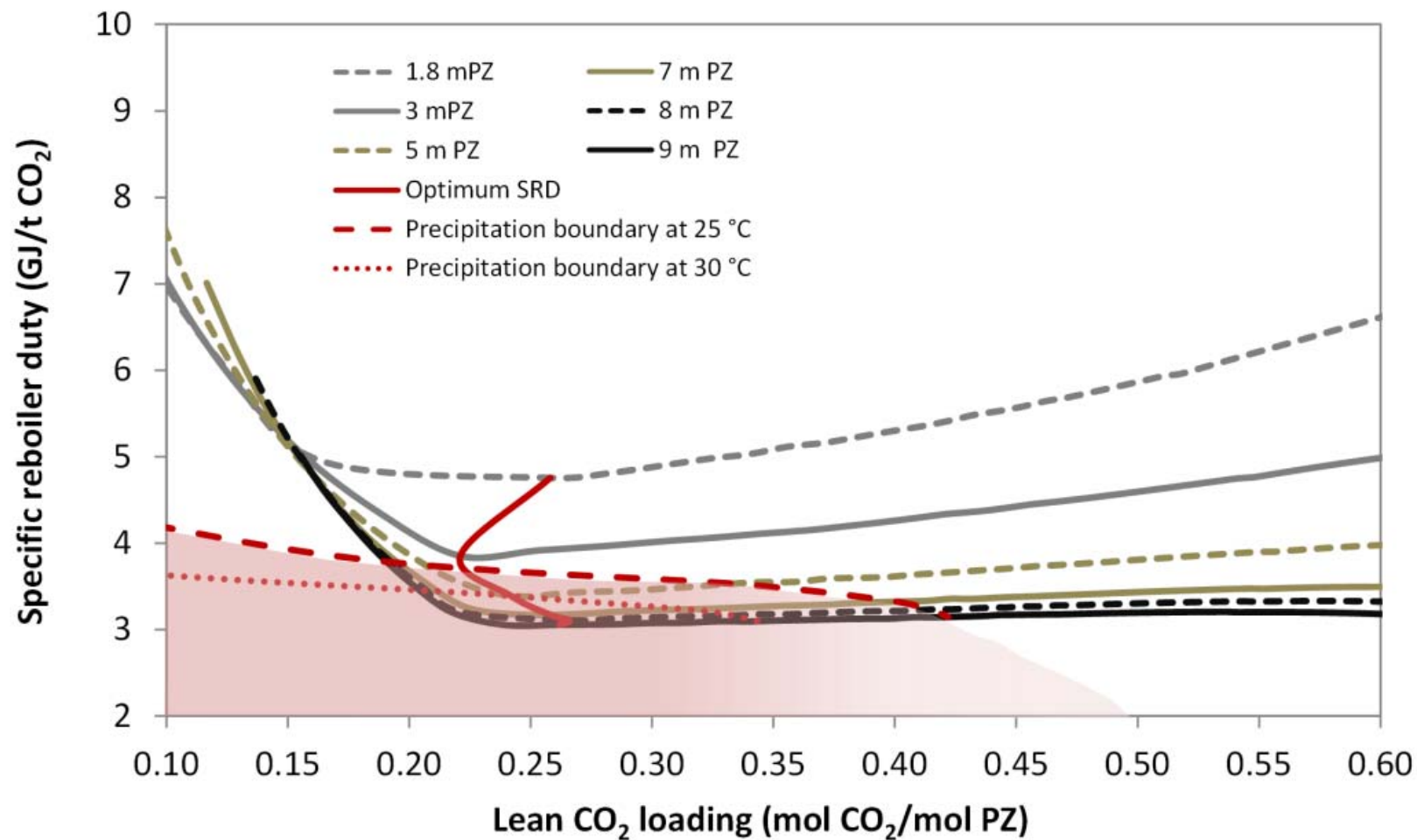
PZ



PZ+K<sub>2</sub>CO<sub>3</sub>

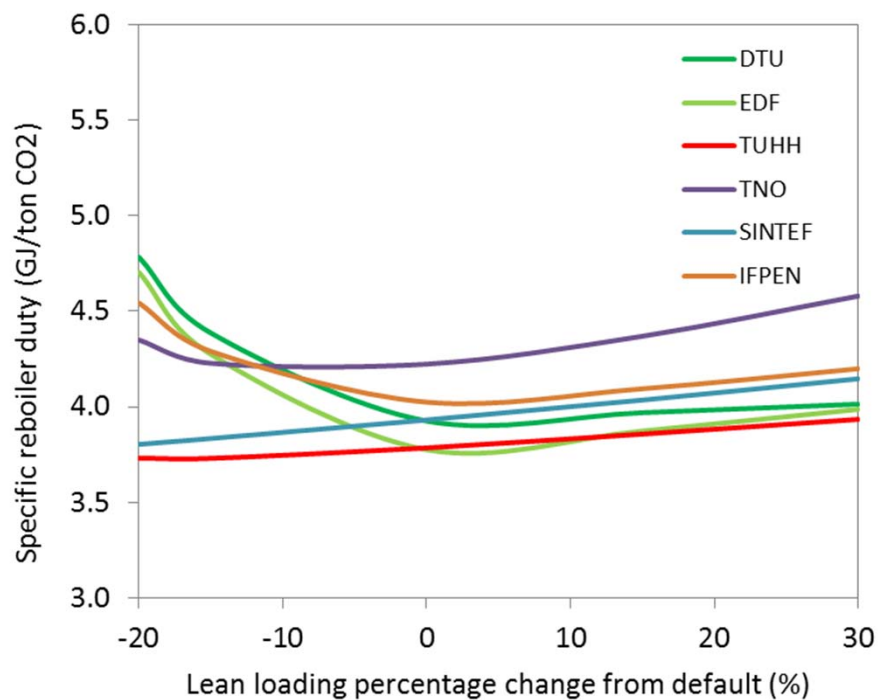


## Rate based simulation with solids (PZ)

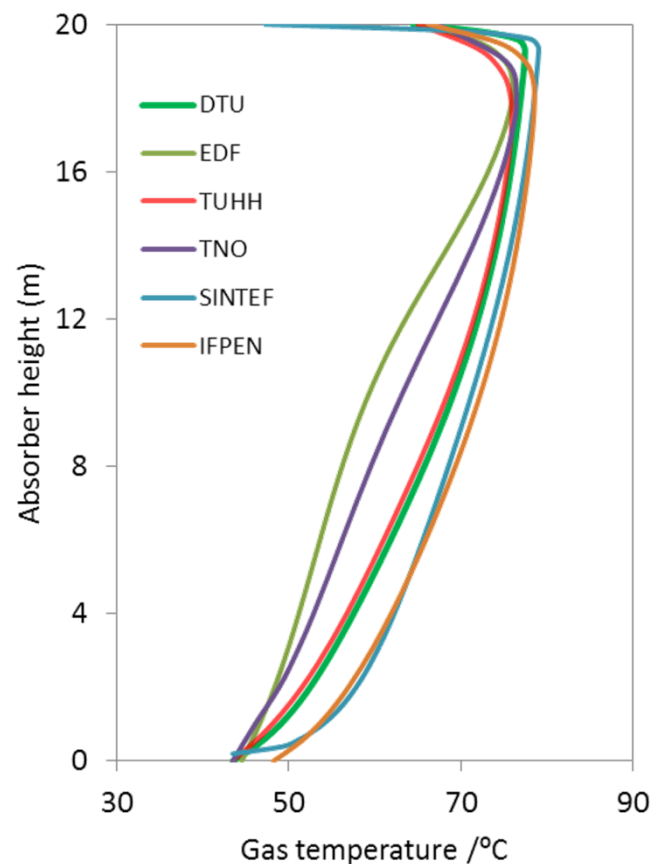


# EU benchmarking

- Desorber reboiler duty
  - Good reproducibility ( $\pm 5\%$ )
  - High scatter at high flooding



- Absorber temperature profiles
  - Midsection scattered ( $10^{\circ}\text{C}$ )
  - Top+bottom high reproducibility ( $1\text{-}5^{\circ}\text{C}$ )

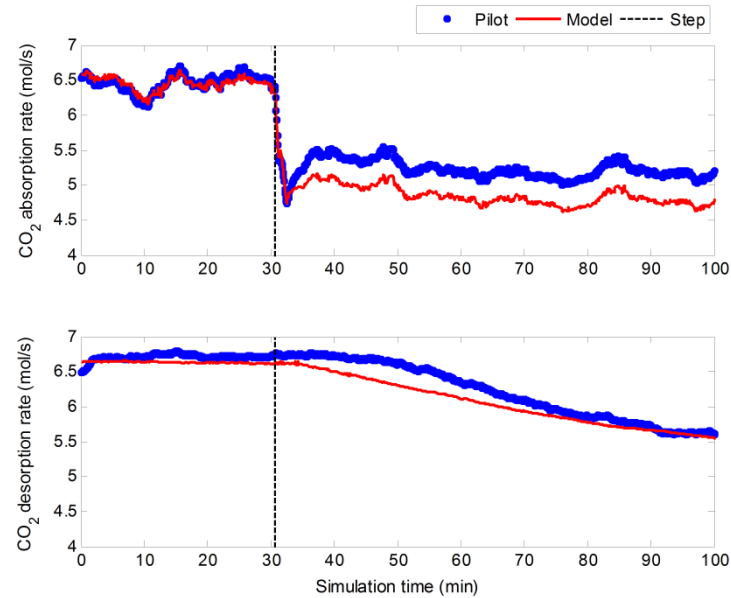
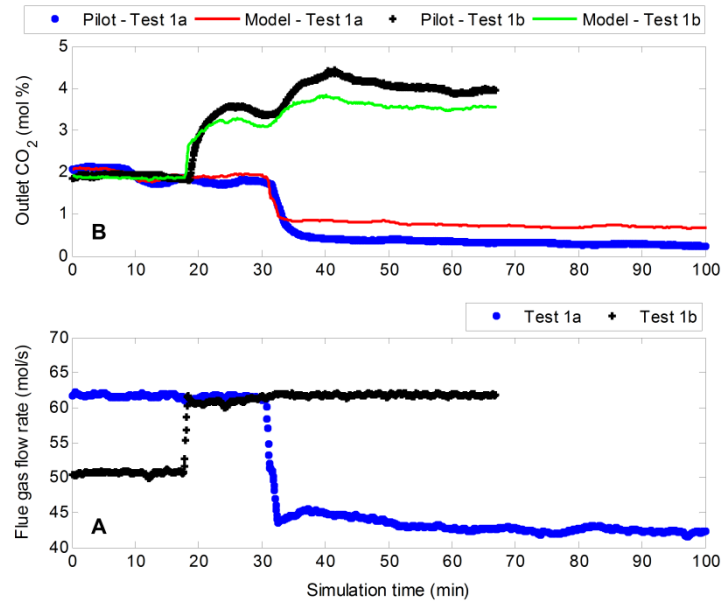




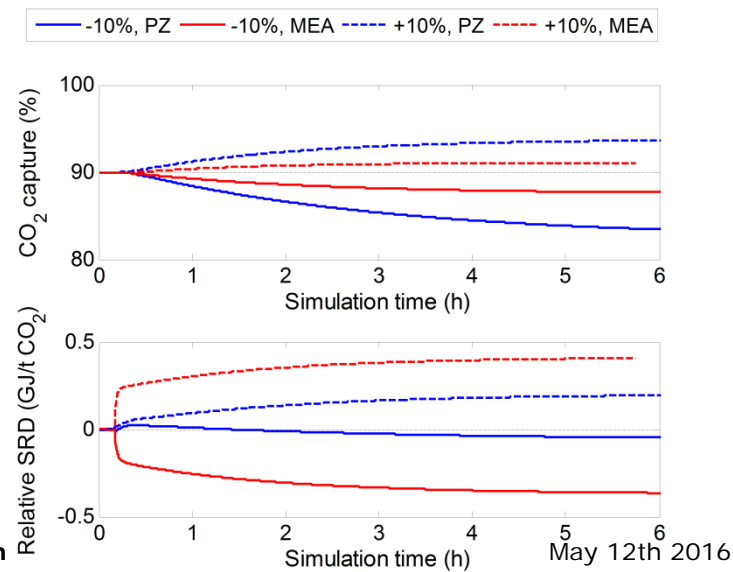
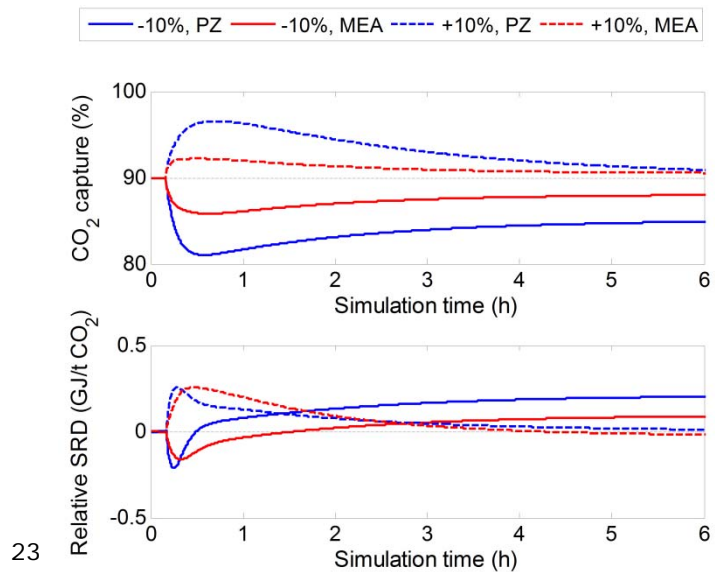
# Dynamic Absorber and Desorber Model



MEA



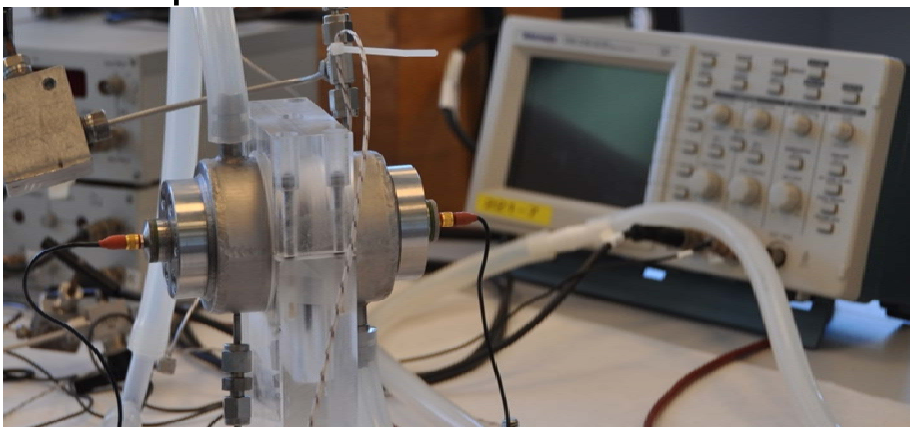
PZ





# Compression & transport

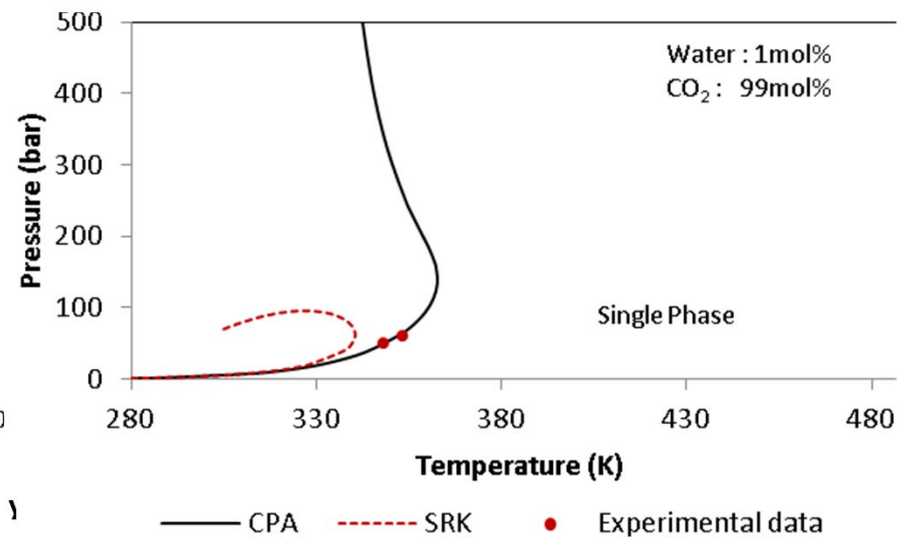
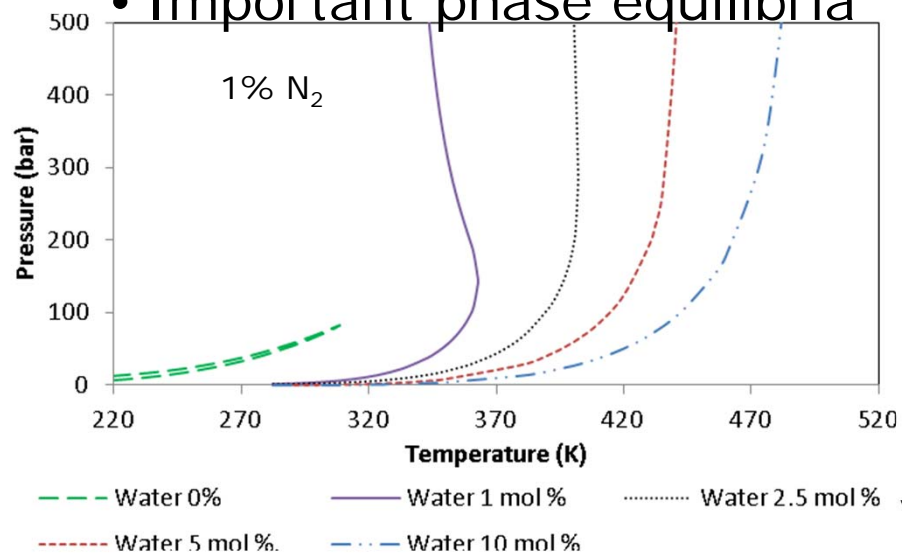
- Speed of sound



- HP Gas diffusion

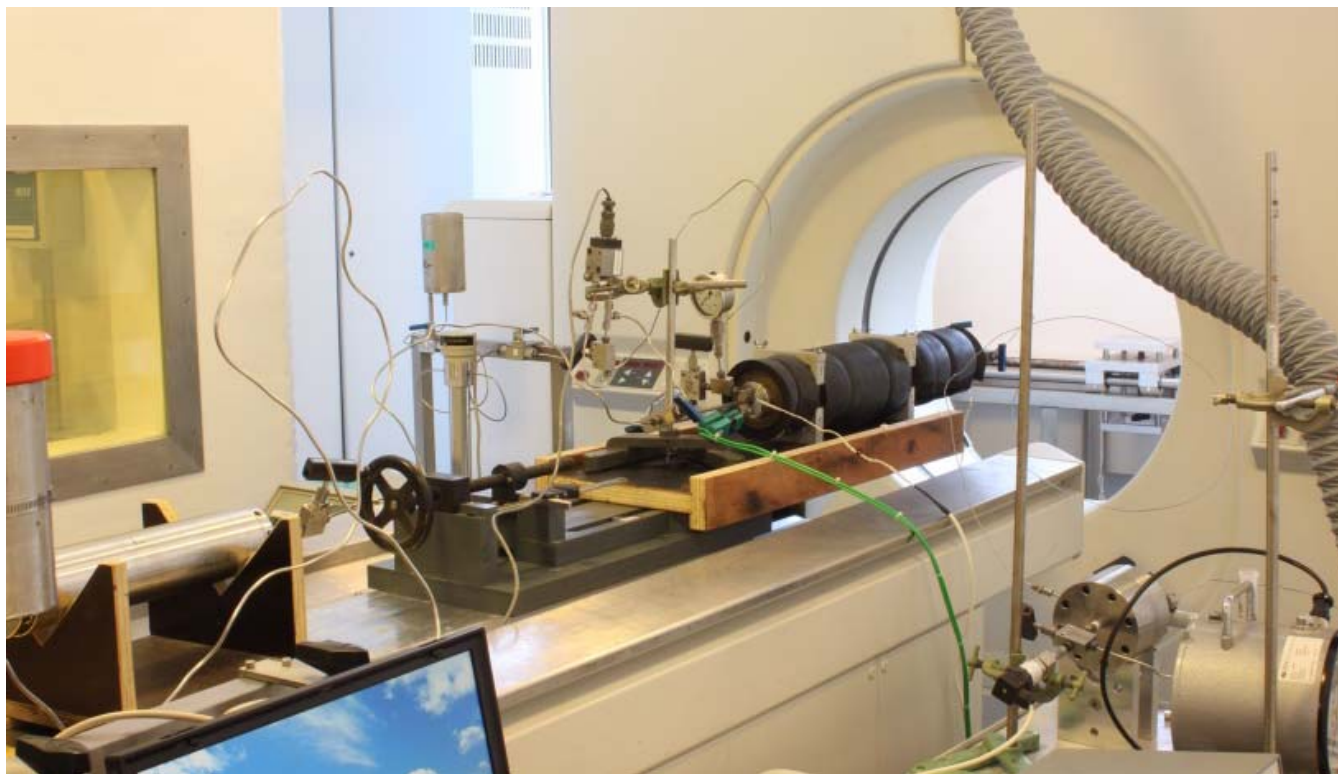


- Important phase equilibria



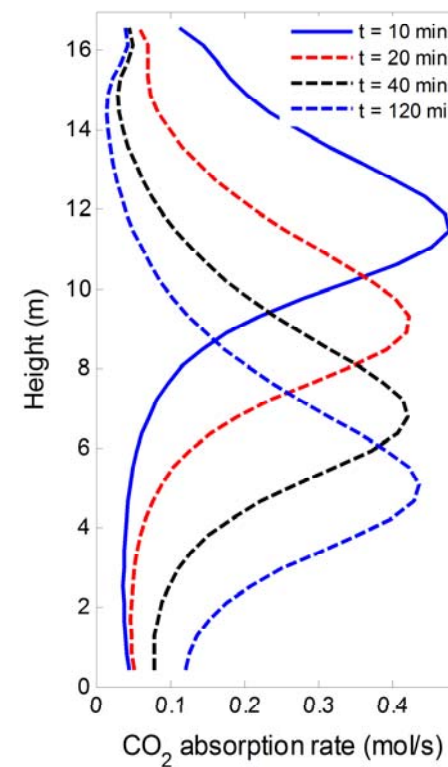
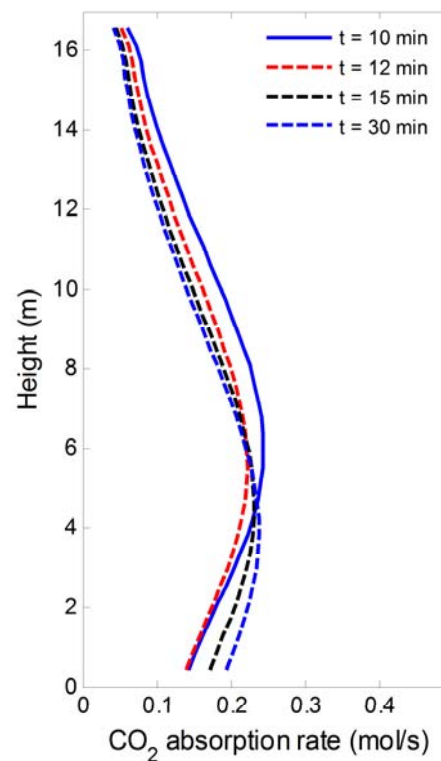
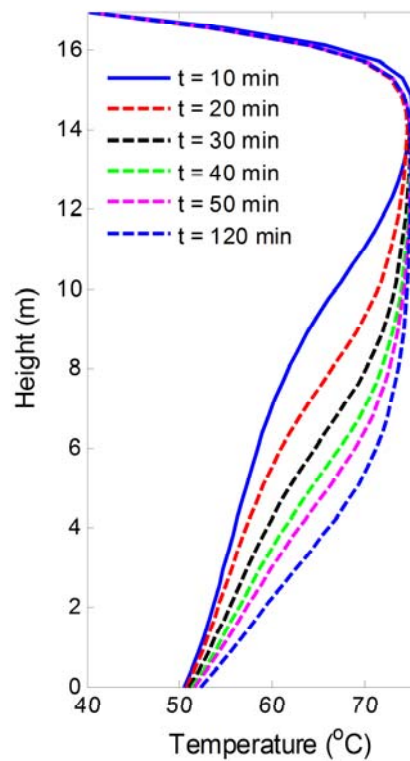
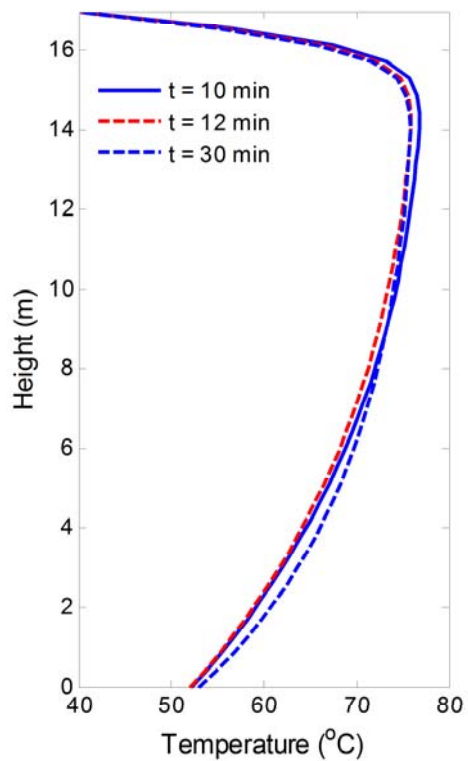
## CO<sub>2</sub> storage

- Reservoir CO<sub>2</sub> injection using CT-scanning

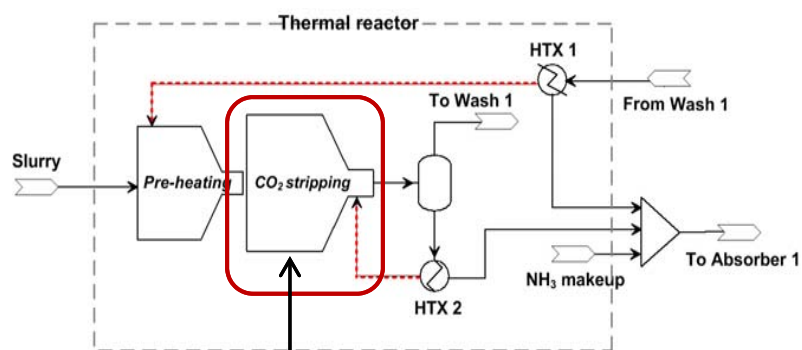




# Dynamics (dCapCO<sub>2</sub>), MEA vs. PZ

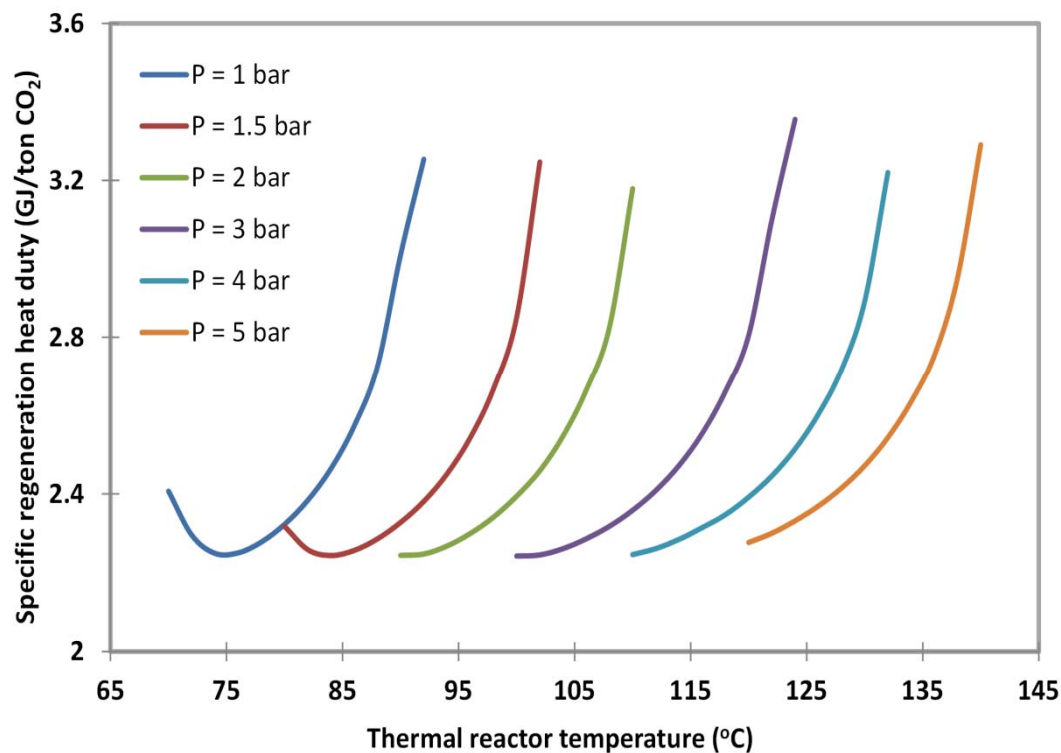


# Optimization of energy consumption



**T = 88  
°C  
P = 1 bar**

**Low- and mid- temperature  
waste/process heat  
integration!**



*Fig. 5. Influence of temperature and pressure on the specific regeneration energy*

## Statements on CO<sub>2</sub> emitting energy sources

- Cheap energy sources **will be used** by 3<sup>rd</sup> world countries as long as they are available
- Coal and oil are **cheap** and **"easy" energy** resources
- **Renewable** technologies will be beneficial for developed countries but will **take longer to implement** in the 3<sup>rd</sup> world
- Several industrial processes produce noticeable amounts of CO<sub>2</sub> which may not be reduced by renewable energy
  - **Cement industry**
  - Fermentation industry (Medicine, food, and bioethanol production)
  - Agriculture
  - Transportation



# CAPCO<sub>2</sub> unit operation

Aspen  
Plus

**a**

Simulation | Main Flowsheet | Control Panel | ABS (DTUCAPCO<sub>2</sub>-UNIQUAC) - Parameters | Setup - Report Options | GAS-FLOW (MATER)

DesignSpecs

Index	Variable	Value	Units	Physical Type
1	DIAMETER	1.1	METER	LENGTH
2	HEIGHT	10	METER	LENGTH
3	CONDENSER_TEMPERATURE	25	C	TEMPERATURE
4	REBOILER_TEMPERATURE	121	C	TEMPERATURE
5	REBOILER_PRESSURE	185000	PA	PRESSURE
6	REBOILER_DUTY	1.01262e+06	J	ENERGY
7	CONDENSER_DUTY	0	J	ENERGY

**b**

Simulation | Main Flowsheet | Control Panel | ABS (DTUCAPCO<sub>2</sub>-UNIQUAC) - Parameters | Setup - Report Options | GAS-FLOW (MATER)

Configuration | UserDefined\_Packing | BuiltIn\_Packing

Name	Value	Description
CONDENSER	None	Configuration of utilities
REBOILER	Internal	Configuration of utilities
MASSTRANSFERMODEL	Rocha, Bravo and Fa...	Mass transfer and hydraulic capacity correlation mo...
ENHANCEMENT_FACTOR	DTU-GM (2015)	Estimation of mass transfer with simultaneous reacti...
PRESSURE_DROP	None	Pressure drop calculation
SET_PACKING_TYPE	User defined	Packing type