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A general column model in CO2SIM for transient modeling of CO_2 absorption processes

Programming methods and code development

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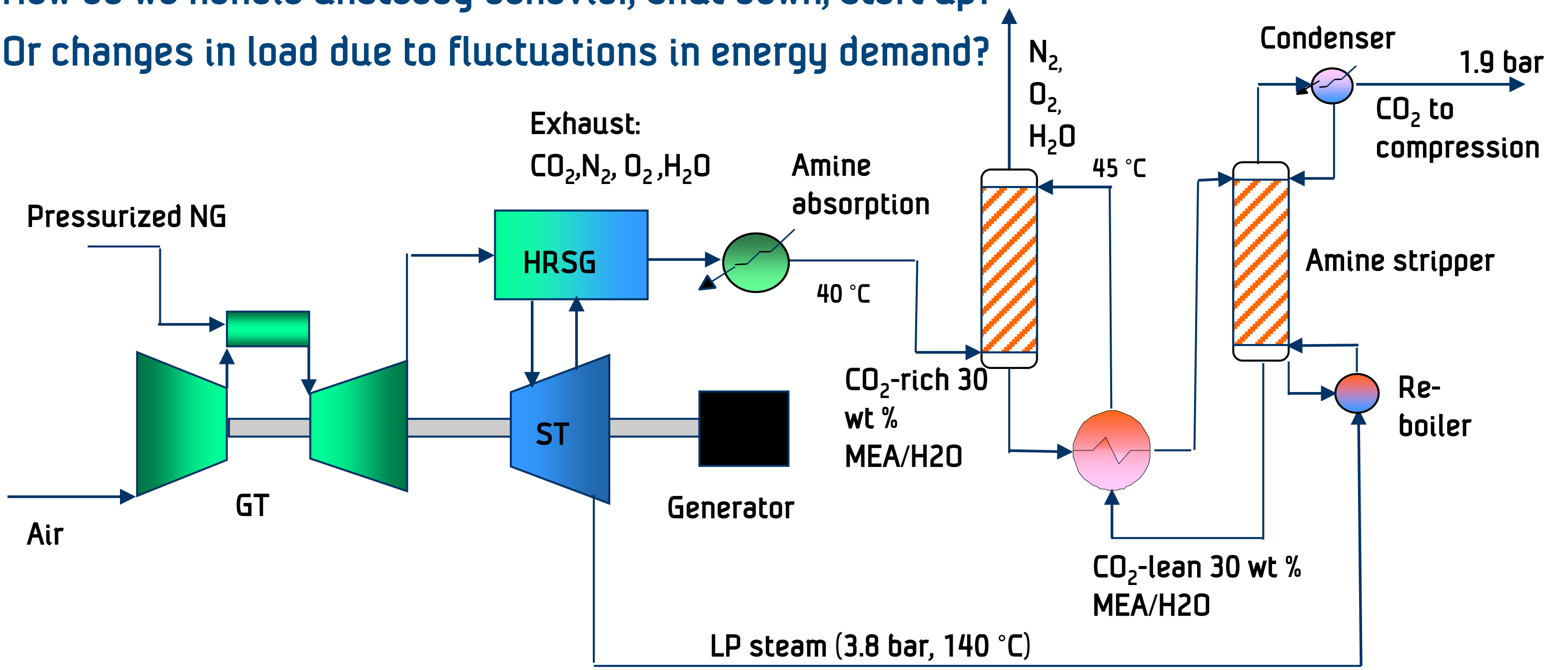
Rationale

- The objective of this work task is to implement a dynamic absorber in CO2SIM
  - The model should be a 'multipurpose' packing model
- Focus is placed on competence building through use of simulation models that can be:
  - verified against experimental and plant data where feedback to the work is done 'fairly quickly' (validation/verification through established routines)
  - by developing dynamic simulation models based on already established computer architecture (efficient development)
- To assist in understanding CO_2 capture processes (or any chemical process), we believe process simulation is beneficial to all phases in a projects lifetime

We are now moving towards building full scale plants

- Large and frequent load changes of the power plant requires understanding of dynamic operation
  - How shall the capture plant be operated and controlled?
  - What are the real consequences of varying loads at the CO_2 removal plant?
  - How do we handle unsteady behavior, shut down, start up?
  - Or changes in load due to fluctuations in energy demand?



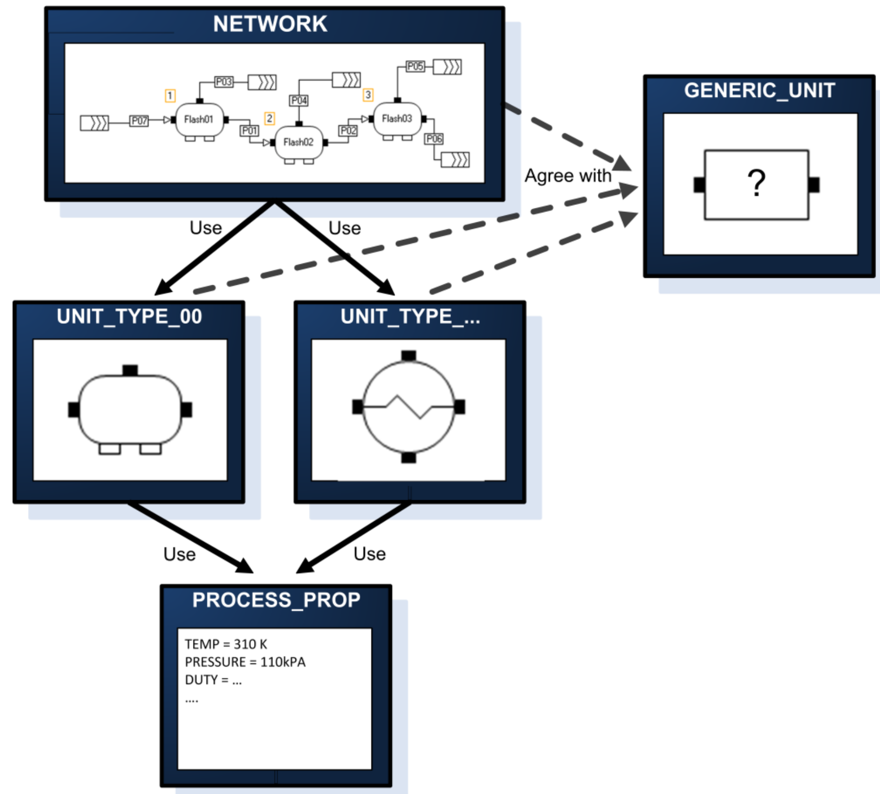
Development Strategy:

- Task 1: Implement a dynamic column model
  - Development of the model for absorption and desorption
  - Test model and validate towards pilot plant data (steady state and dynamic)
- Task 2: Develop the connected unit operations, flash tanks, mixers, storage tanks and heat exchangers
  - Definition of unit operations built into CO2SIM
- Task3: Develop the dynamic Network solver
  - Flowsheet model
  - Programming techniques: information handling
  - Information structure
    - relationship between an event (the cause) and a second event (the effect) -> causality

This work is extensive…
Our first requirement is therefore: We must have a *platform* for development

CO2SIM programming techniques

- *Fundamental problem:* Exponential increase in complexity as code becomes larger
- Requires focus on structural planning and architectural patterns
  - *Design patterns* can speed up the development process
  - Provides fundamental development methods related to
    - program organization
    - and common data structures (classes)
  - *In other words; the basic code elements at each layer are reusable*
  - The code design should be general enough to address future requirements also



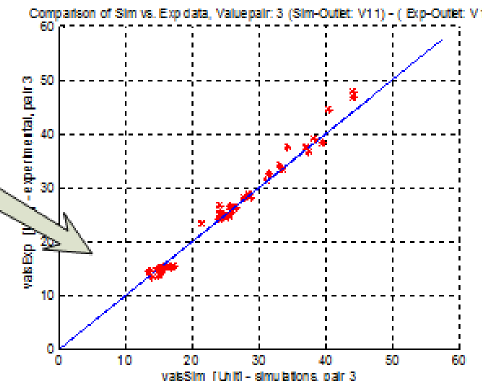
Such design patterns provide general solutions, documented in a format that does not require specific ties to a particular problem

Example: Use of 'Design patterns' does generalize code development

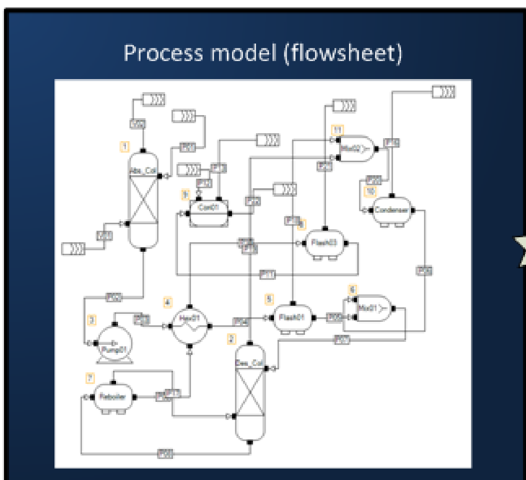
Test facility

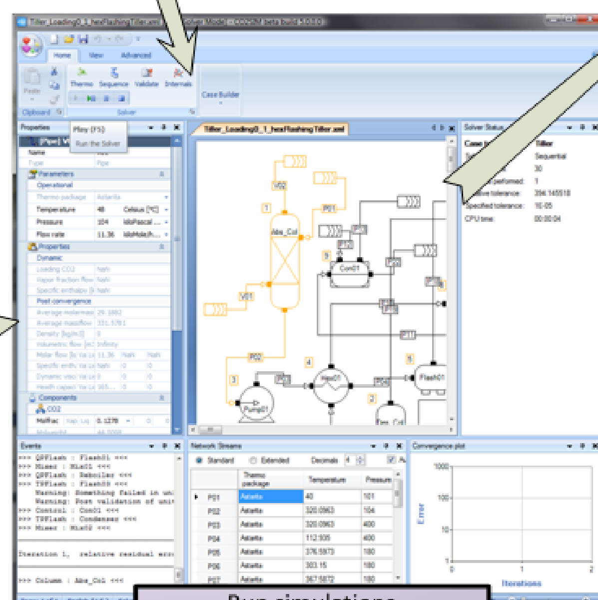
	A	B	C
1	Parameter/measurement	Unit	Value
2	Streams for absorber		
3	V1 Tag		V1 Inlet Absorber
4	V1 Temp	C	46.16147749
5	V1 Press	kPa	103.9904464
6	V1 Flow	kmol/h	9.792997189
7	V1 molfrac CO2	[]	0.03909028
8	V1 molfrac H2O	[]	0.069868751
9	V1 molfrac Amine	[]	0
10	V1 molfrac Inerts	[]	0.891040969

Register experiment outputs



Evaluate and compare



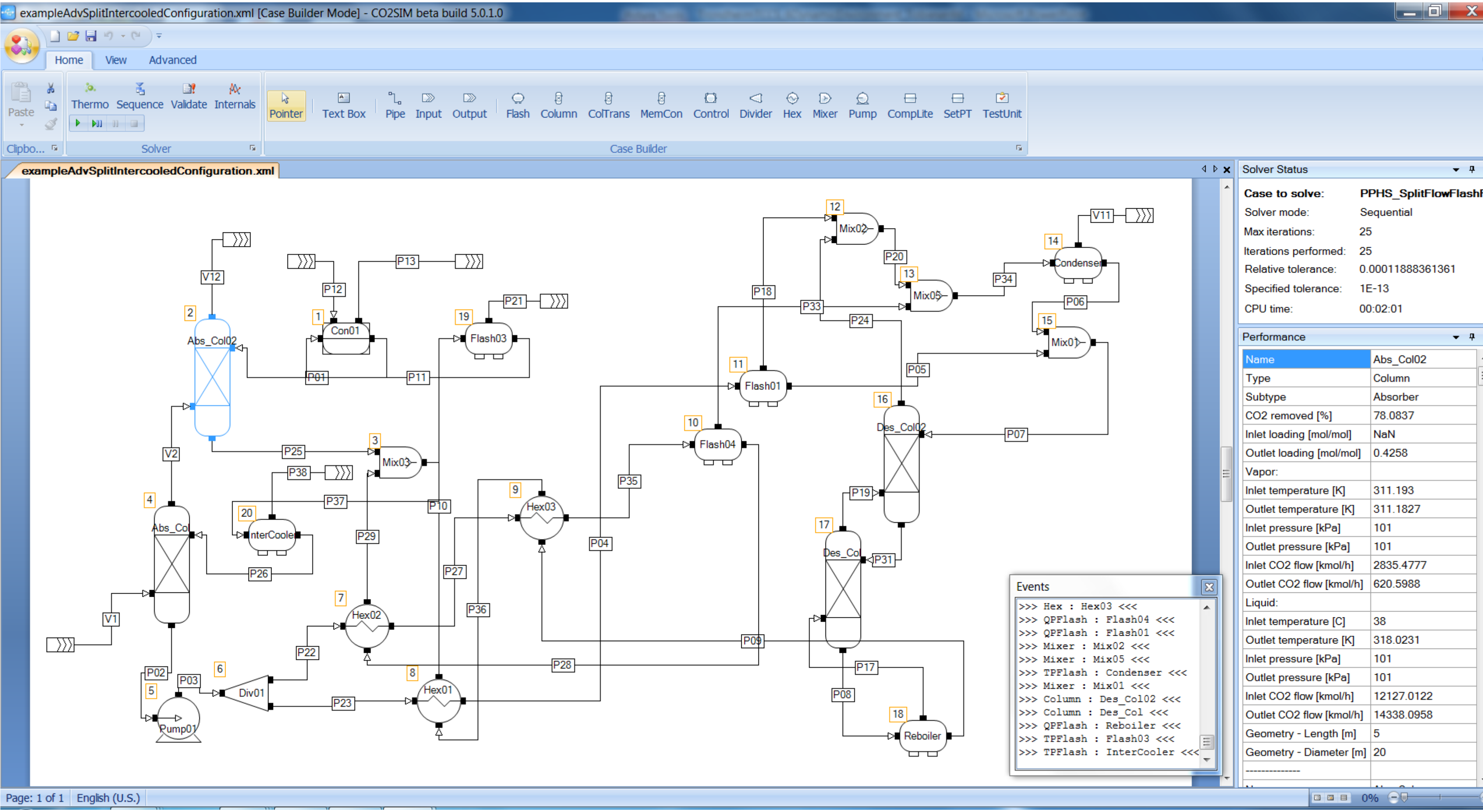


Run simulations

Routine that minimizes the need for manually processing data

1. Obtain plant data for the full campaign
2. Duplicate plant flow sheet in the simulator
3. Simulate the complete campaign (one execution)
4. Evaluate statistics for the full campaign
5. Further use: optimization etc.

Development platform CO_2SIM@SteadyState

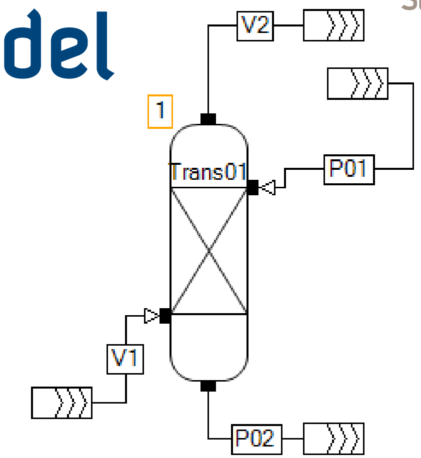


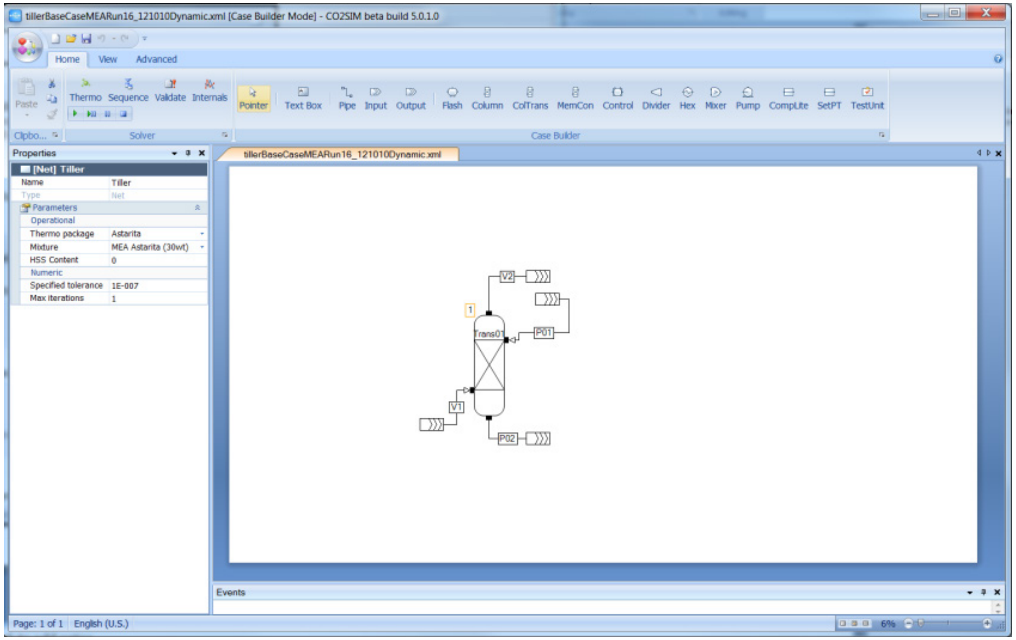
Development Strategy

- Task 1: Implement a dynamic CO2SIM column model
  - Model description and numerical methods
  - Test model and validate towards pilot plant data (steady state and dynamic)
- Task 2: Develop the connected unit operations, flash tanks, mixers, storage tanks and heat exchangers
  - Definition of unit operations built into CO2SIM
- Task3: Develop the dynamic Network solver
  - Flowsheet model
  - Programming techniques: information handling
  - Information structure:
    - relationship between an event (the cause) and a second event (the effect) -> causality

Task 1: The transient column model

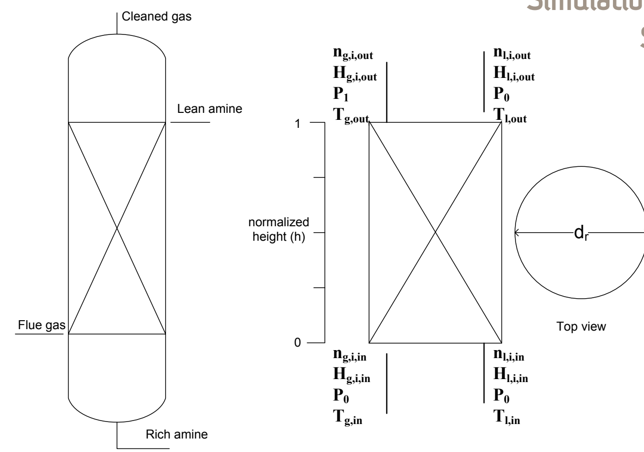
- Based on first principle conservation laws for energy and mass
- Adaptability of the code for different chemical systems and process configurations have been emphasized





The transient column model

Transport equations



Gas phase

$$\varepsilon_G C_{tot,G} \frac{\partial y_i}{\partial t} = -n_{tot,G} \frac{1}{L} \frac{\partial y_i}{\partial z_n} - \left(N_i a - y_i \sum_j N_j a \right)$$

$$\frac{dn_{tot,G}}{dz} = -\sum_j N_j a + \frac{d(\varepsilon_G C_G)}{dt}$$

$$\varepsilon_G \frac{\partial T_G}{\partial t} = -u_G \frac{1}{L} \frac{\partial T_G}{\partial z_n} - \frac{a}{\sum_i (C_i C_{p,i})_G} \cdot h_{G/L} \left(T_L - T_G \right)$$

Liquid phase

$$\varepsilon_L C_L \frac{\partial x_i}{\partial t} = n_{tot,L} \frac{1}{L} \frac{\partial x_i}{\partial z_n} + \left(N_i a - x_i \sum_j N_j a \right)$$

$$\frac{dn_{tot,L}}{dz} = -\sum_j N_j a$$

$$\varepsilon_l \frac{dT_L}{dt} = -u_L \frac{1}{L} \frac{\partial T_L}{\partial z_n} - \frac{a}{\sum_i (C_i C_{p,i})_L} \left(h_{L/G}(T_L - T_G) - \sum_j \Delta H_j N_j - H_{wall}(T_L - T_{out}) \right)$$

Bondary conditions

$$y_i(z_{n,0}) = y_{i,\text{feed}} \qquad x_i(z_{n,1}) = x_{i,\text{feed}}$$

$$n_{tot,G}(z_{n,0}) = n_{tot,G,feed} \qquad n_{tot,G}(z_{n,1}) = n_{tot,feed}$$

$$T_G(z_{n,0}) = T_{G,feed} \qquad T_L(z_{n,1}) = T_{L,feed}$$

$C_G = P/(RT_G)$ **Ideal gas or SRK model**

$n_{tot} = mol/m^2/s$

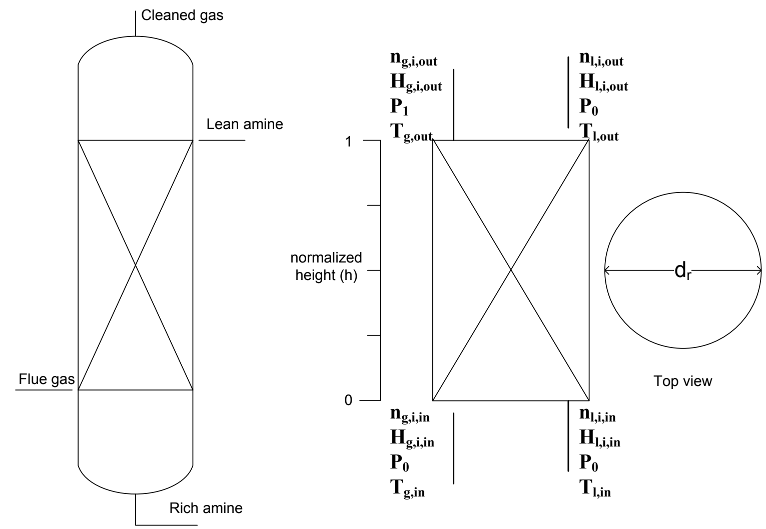
$z_n = z/L$ **normalized column lenth**

An extension of the model presented in: *Kvamsdal, Jakobsen and Hoff, Chemical Engineering and Processing:, Volume 48, Issue 1, January 2009*

The transient column: numerics

Numerical solution to stiff DAE's

- Two point differential algebraic problem (DAE) in a single dimension
- Discretization
  - *Time*
    - Higher order integrator
  - *Space*
    - Static collocation derivatives
- To increase robustness we need
- Stabilizing methods
  1. Normalization
  2. Dynamic relaxation (gives initial steadystate slopes)

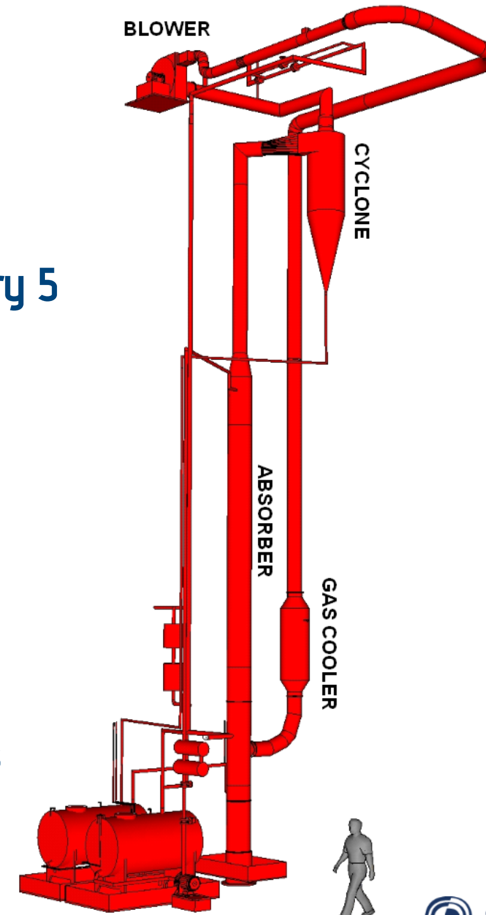


Outline

- Dynamic modeling of CO_2 absorption plants
- Project description
  - Simulator requirements/capabilities
  - Short description of simulation model
- **Verification/Validation (Preliminary)**
  - **Experimental validation using pilot plant data**
- Simulation studies
  - Ramp behavior
  - Robustness of code
- Summary
- Further work
- Acknowledgements

Experimental validation of dynamic column model

- Tested against the "VOCC rig"
- Two time series cases (case A and B)
- 30wt%MEA
- Logging of input and output data every 5 seconds
  - The cases give about 500 updates during simulation
- CO2SIM handles all these "events" automatically during integration to reflect process changes.
  - The events are collected and systematically handled from log files (excel).

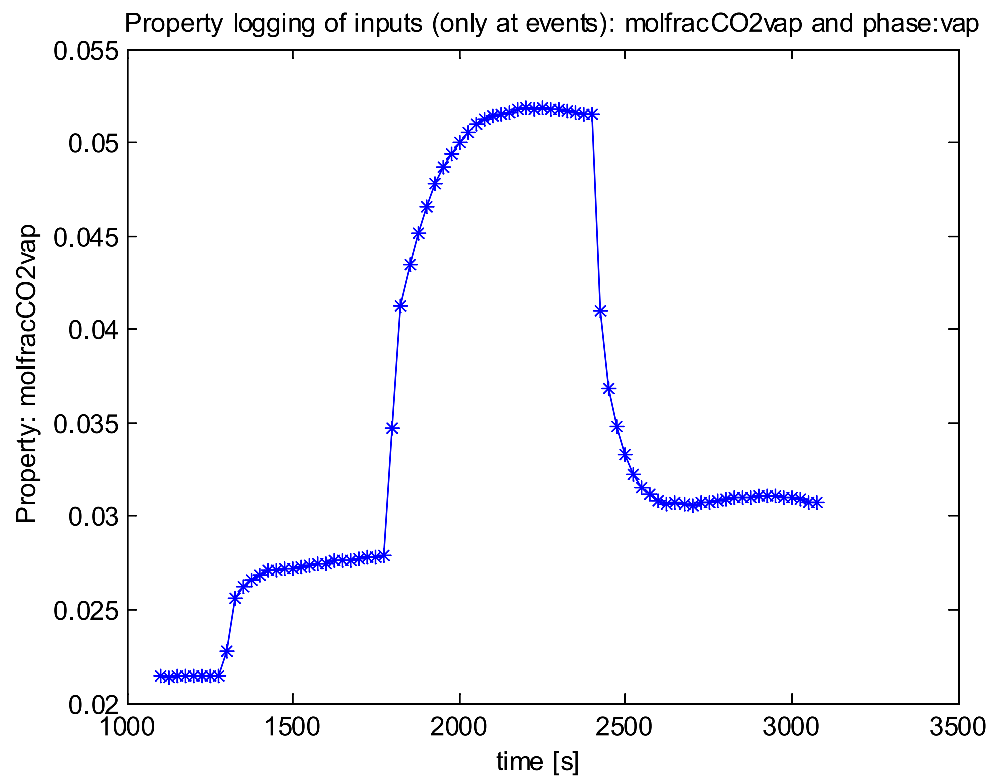


Absorber:
Packing height = 5.4m
ID = 0.5m

Validation of CO2 Capture - The VOCC-project (2007)

VOCC test case

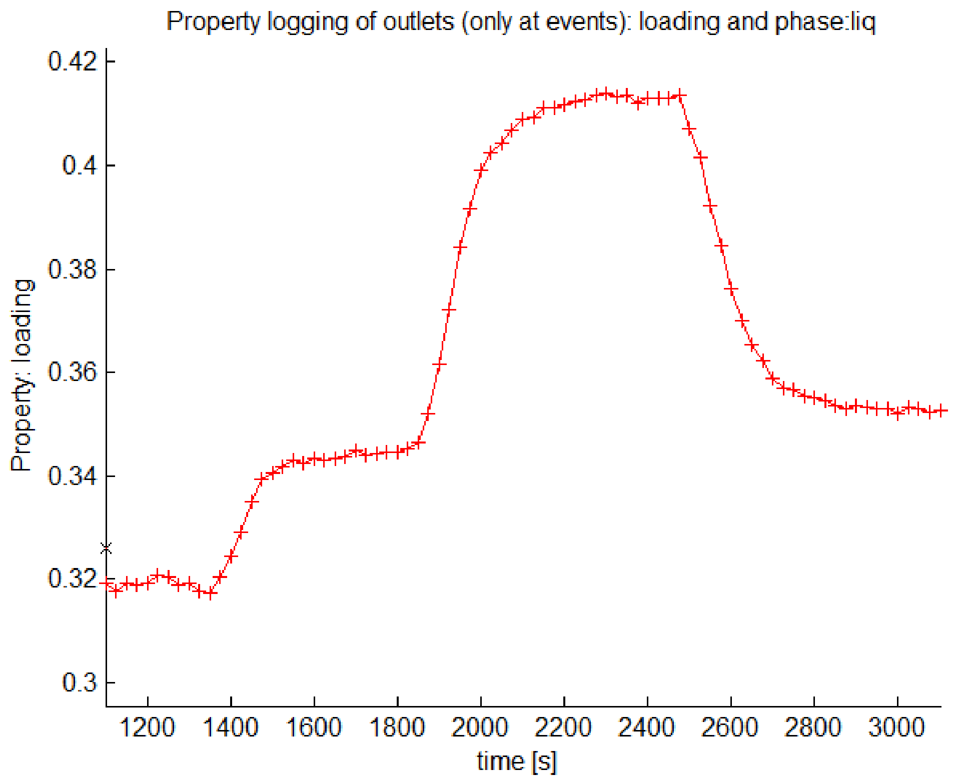
- Case B: Stepwise variations in CO_2 gas concentration
  - Inlet gas concentration of CO_2 increased in two single step-changes
  - then decreased in a large reverse single step-change
  - All other process variables kept constant
    - ✓ Stable liquid and gas flow over the experiment.



Comparing data from VOCC test with simulation

Simulated and measured:

Rich loading

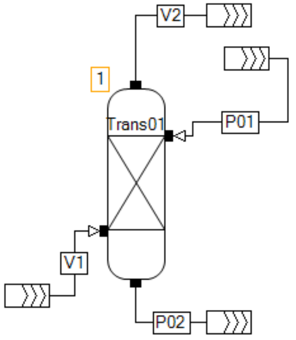


Red line – PILOT data

Blue line – SIMULATION

Simulation time increased 30 times

20-30 times faster than real-time



Comparing data from VOCC test with simulation

Simulated and measured:

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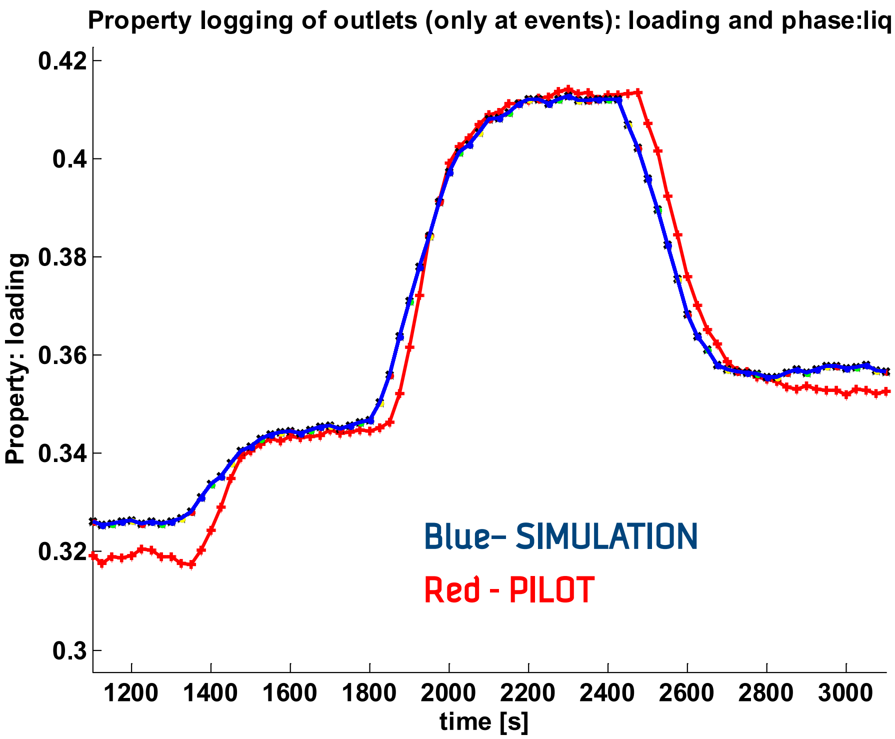
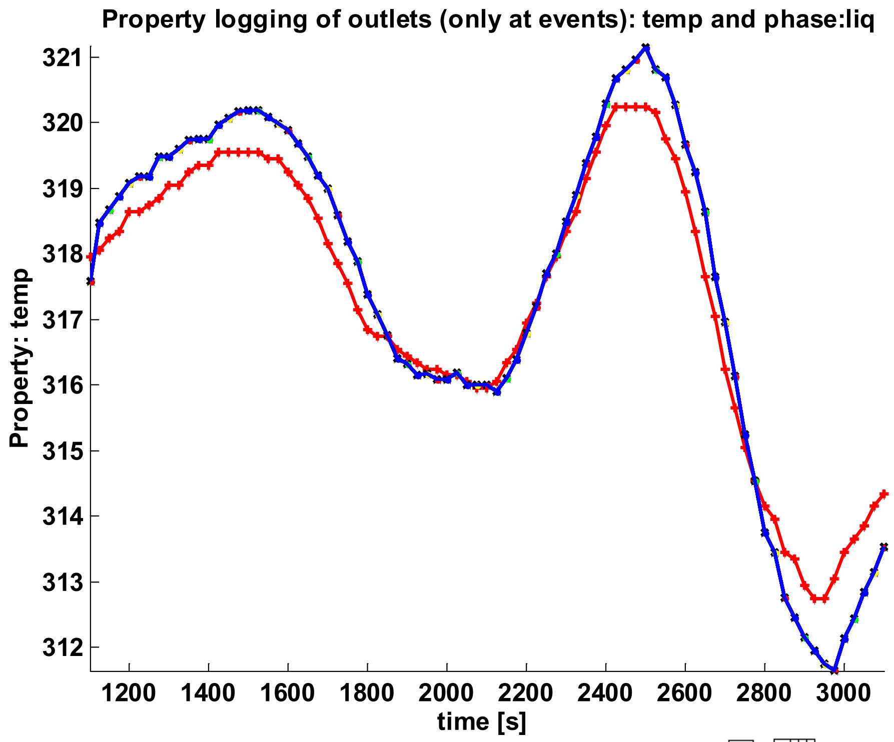
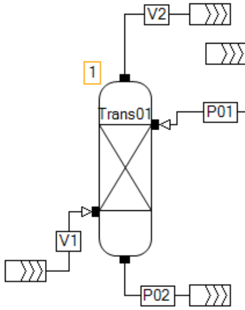


Simulated and measured:

Outlet Liquid Solvent temperature



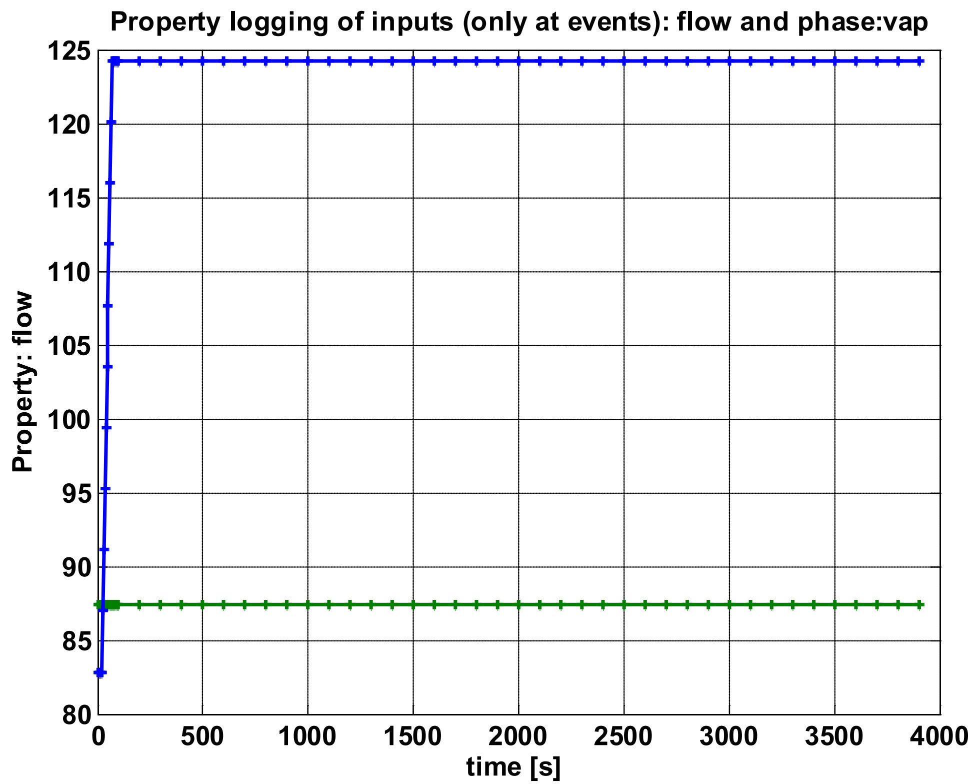


Simulation example

Case A: Increasing gas load

- Increasing molar ratio between the gas and liquid flowrate
  - Varying the liquid and vapor input flow rates by ~50%?
    - In a time frame of 50 seconds
  - Initially running at steady state then increase gas flow with 50% over a short time interval
  - Observe the transients, then run end situation to steady state again

- 20 meter packing, identical inlet concentrations , only vary flow rate

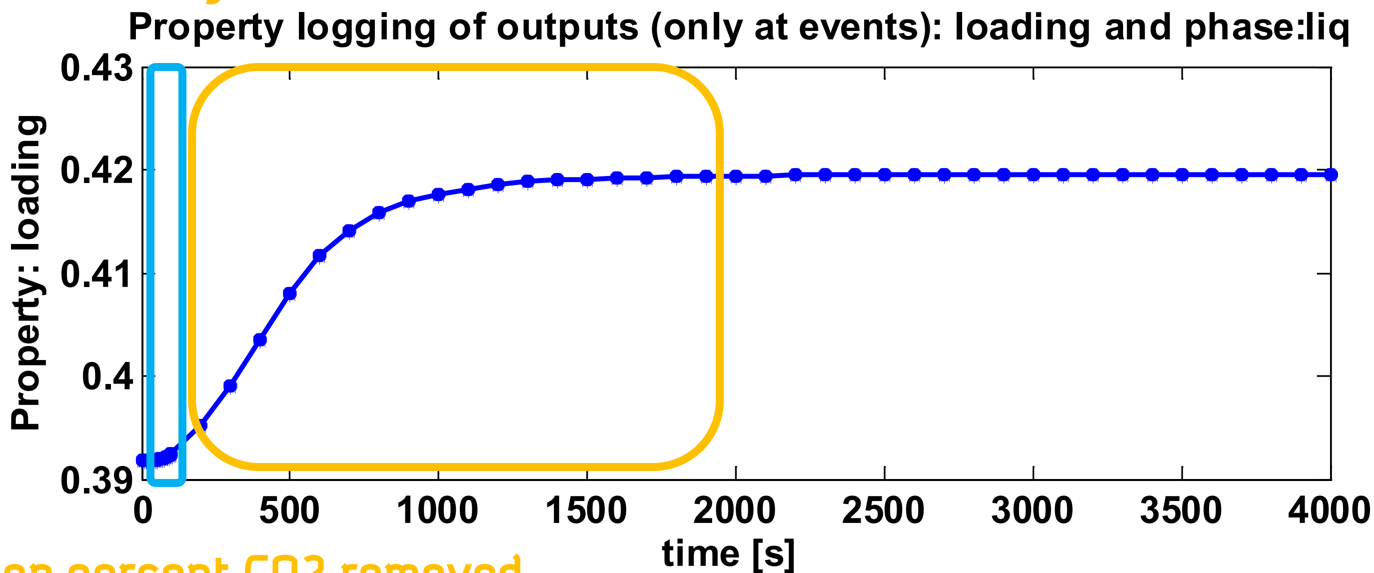


Blue: gas flowrate (kmol/h)

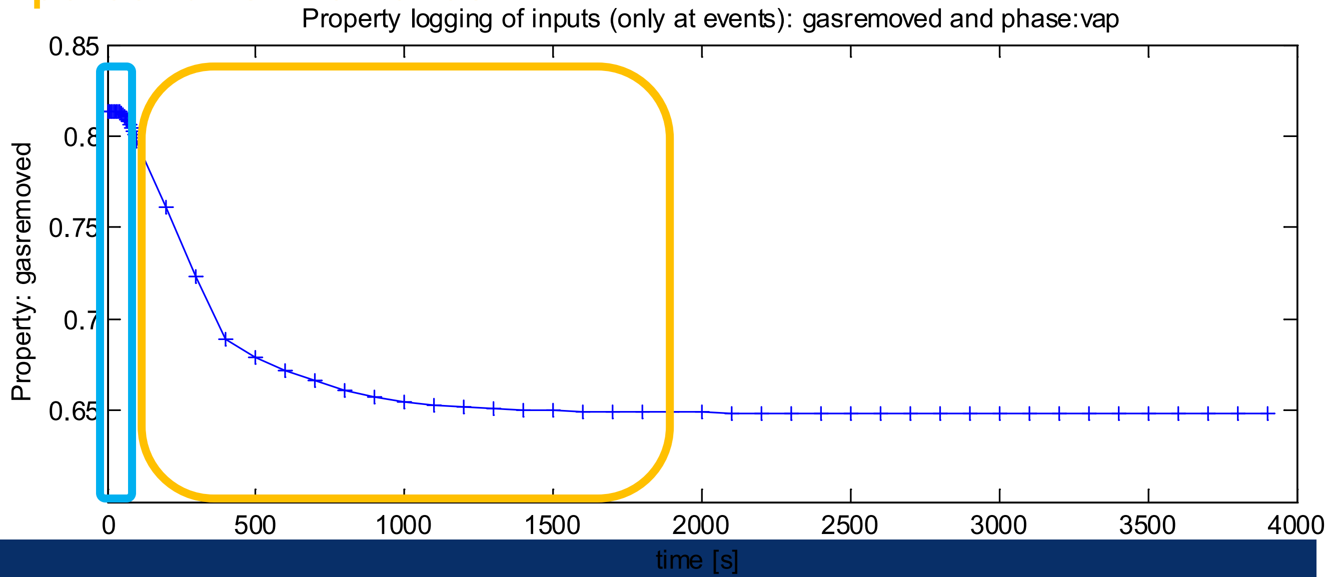
Green: liquid flow rate (kmol/h)

Case A: Increasing the flue gas load

Effect on loading

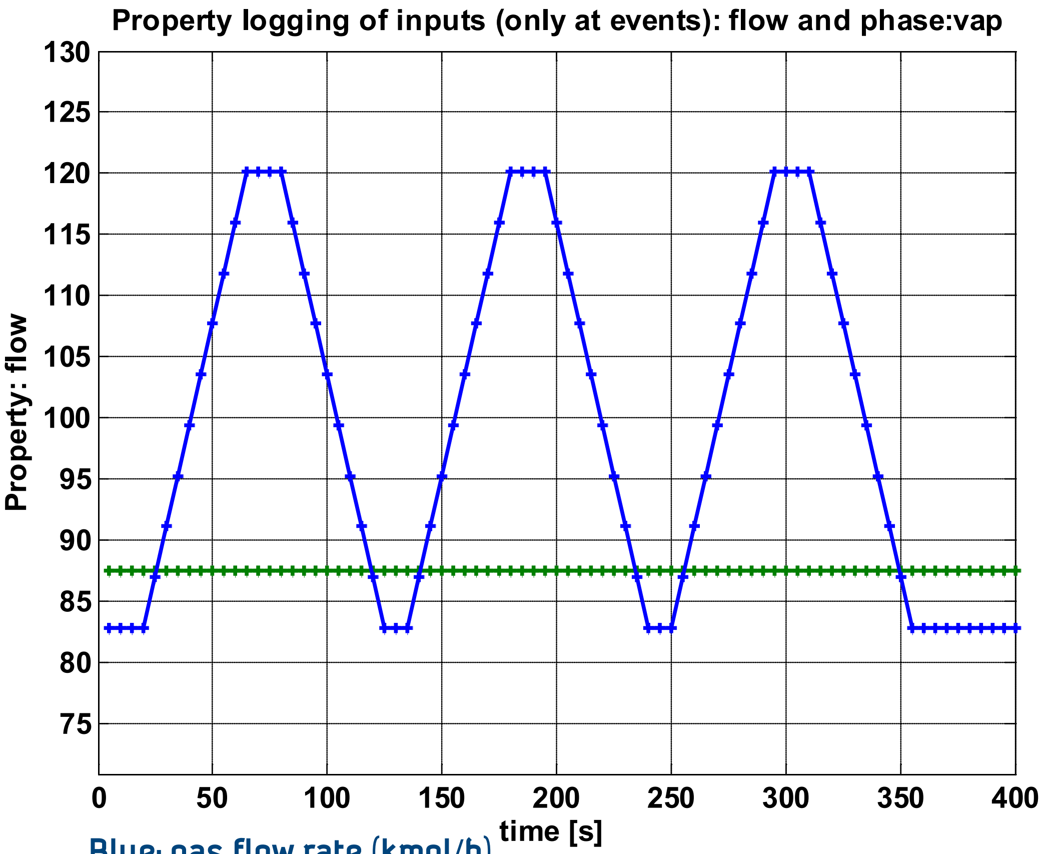


Effect on percent CO2 removed



Case B: Varying flue gas load

- Varying the molar ratio between the gas and liquid flow rate
  - In a time frame of ~300 seconds
  - Initially running at steady state then increase/reduce gas flow with 50%
  - Observe the transients, then run end situation to steady state again
- 20 meter packing, identical inlet concentrations , only vary flow rate

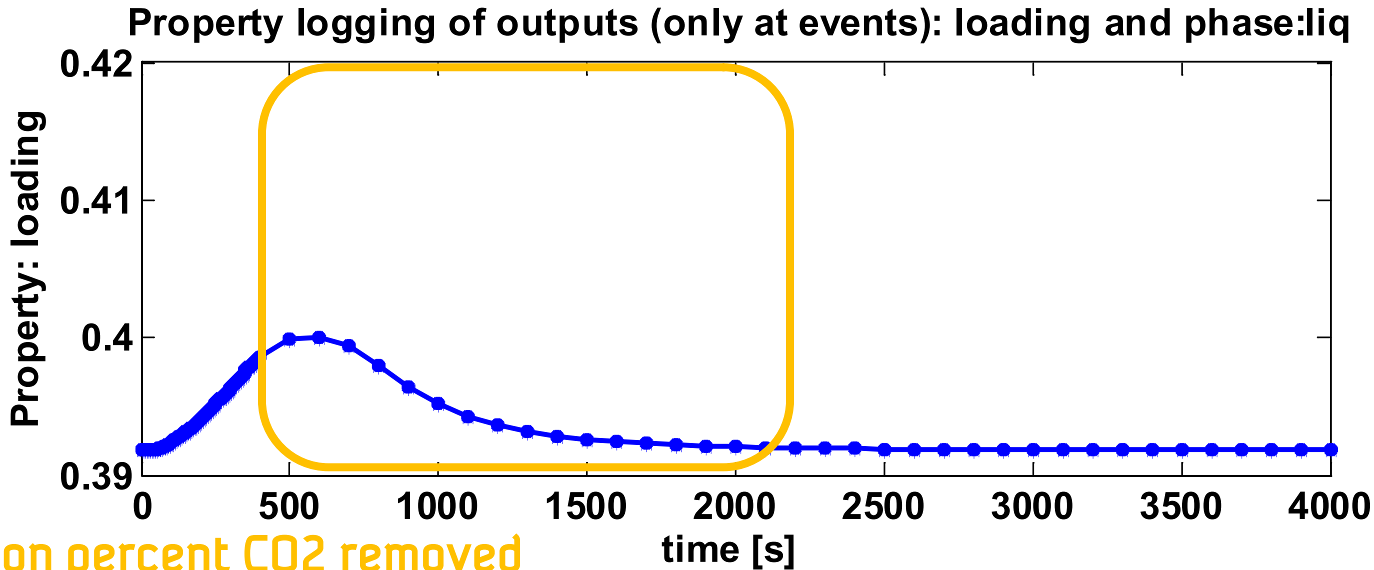


Blue: gas flow rate (kmol/h)

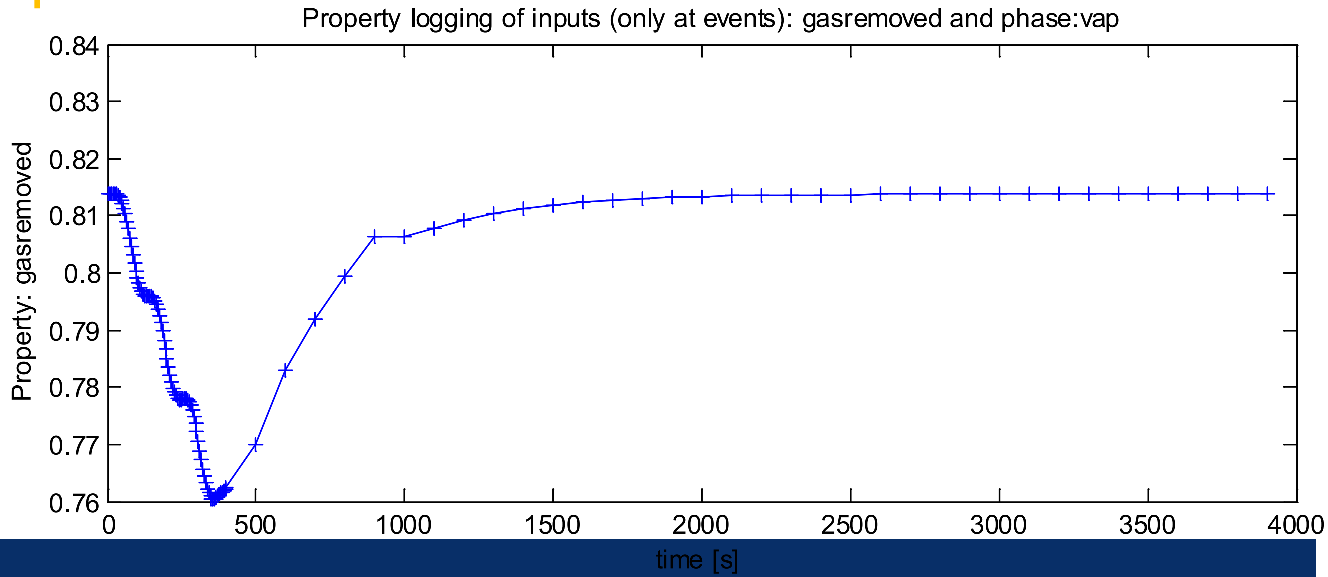
Green: liquid flow rate (kmol/h)

Case B: Varying the flue gas load

Effect on loading



Effect on percent CO2 removed

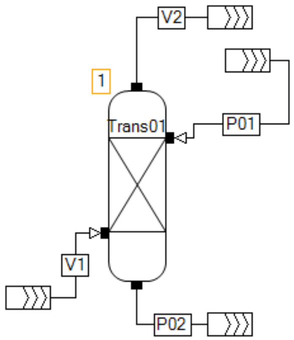


Summary

- At this stage in the project a robust codebase is developed for dynamic simulation
  - Absorber, desorber packing model (this presentation)
    - Verified numerics
    - Validated towards plant data (preliminary)
- The event updating procedures facilitates rapid simulation using plant data for validation
- Current model gives acceptable match towards data for MEA
  - Both at dynamic and steady state operation
- The implementation methodology allows for efficient simulation of the units' transient behavior for continuously changes in input conditions or design parameters, part load operation, varying input conditions and ramping behavior

Further work

- A few units implemented: Storage tank, dynamic flash, mixer tank and the column model
- Network solver to handle sequential dynamic integration



Acknowledgement

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