NETL Crosscutting Research Portfolio Review
Pittsburgh, PA
22nd March 2017

Commercialization Potential of Carbon Capture Simulation Initiative (CCSI) Tools

Award Number FE0026307

Adekola Lawal

Outline

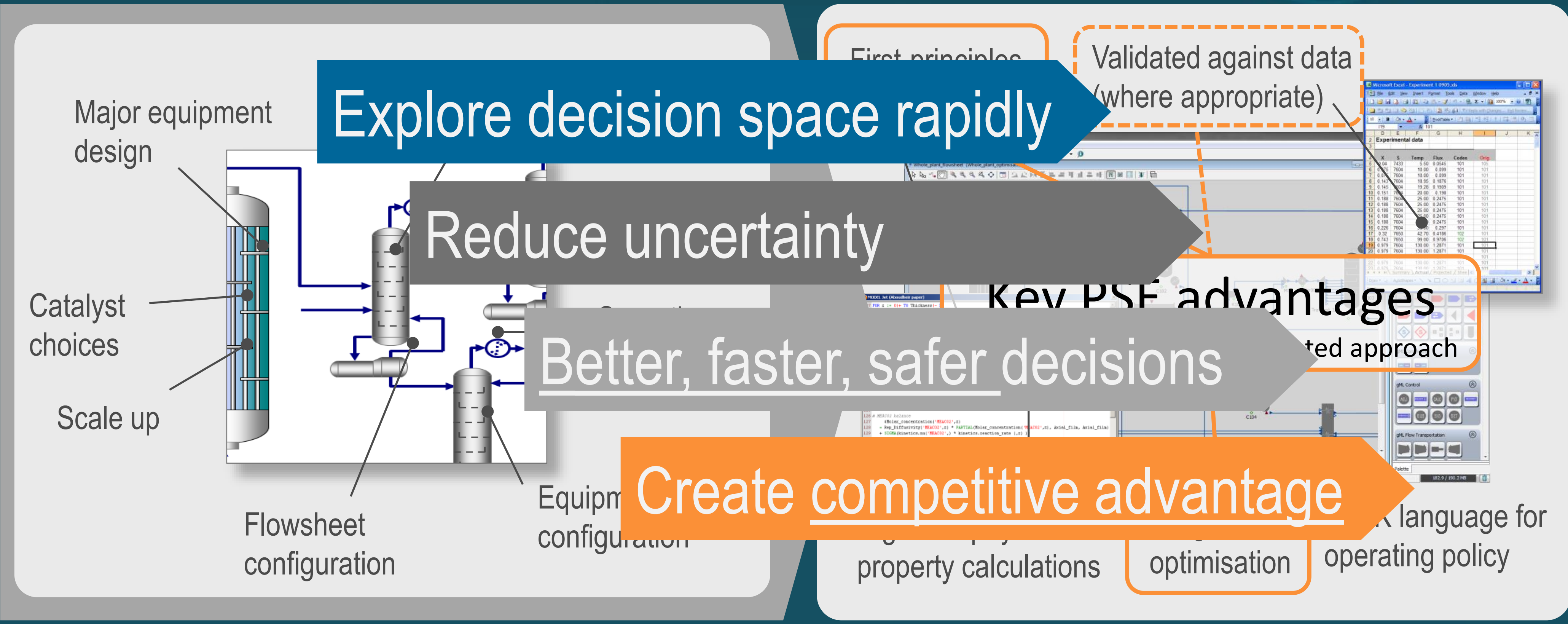
- Making the case for advanced process modelling
- PSE background
- CCSI Toolset Commercialization Project
  - Background
  - Project Overview
  - Screening and assessments
  - Case studies: Improving commercial potential
- Summary

ADVANCED PROCESS MODELLING

A combination of *high-fidelity modelling*, *advanced optimisation* and *system analysis* techniques within an *equation-oriented* framework

Decisions, decisions …

… based on accurate predictive models



PSE BACKGROUND: FROM RESEARCH TO INDUSTRY

1997

Company 'spun out' of Imperial College
Private, independent company incorporated in UK

gPROMS

Acquires technology

2007

PSE wins Royal Academy MacRobert Award for Engineering Innovation. This is the UK's highest engineering award

Now

International company delivering software and services

Major industry focus

Strong R&D

Established sectors

- Chemicals & Petrochemicals
- Oil & Gas
- Formulated Products

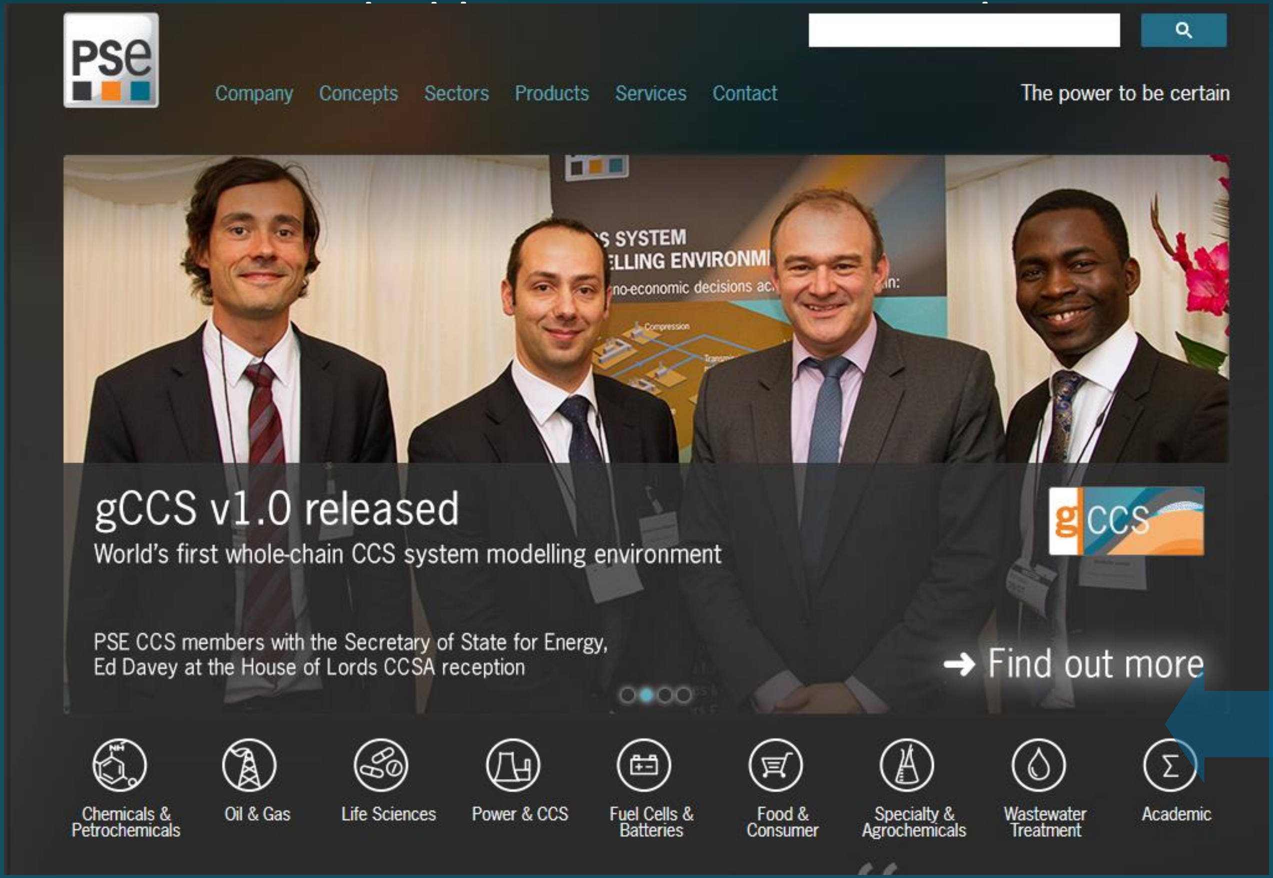
Strategic initiatives

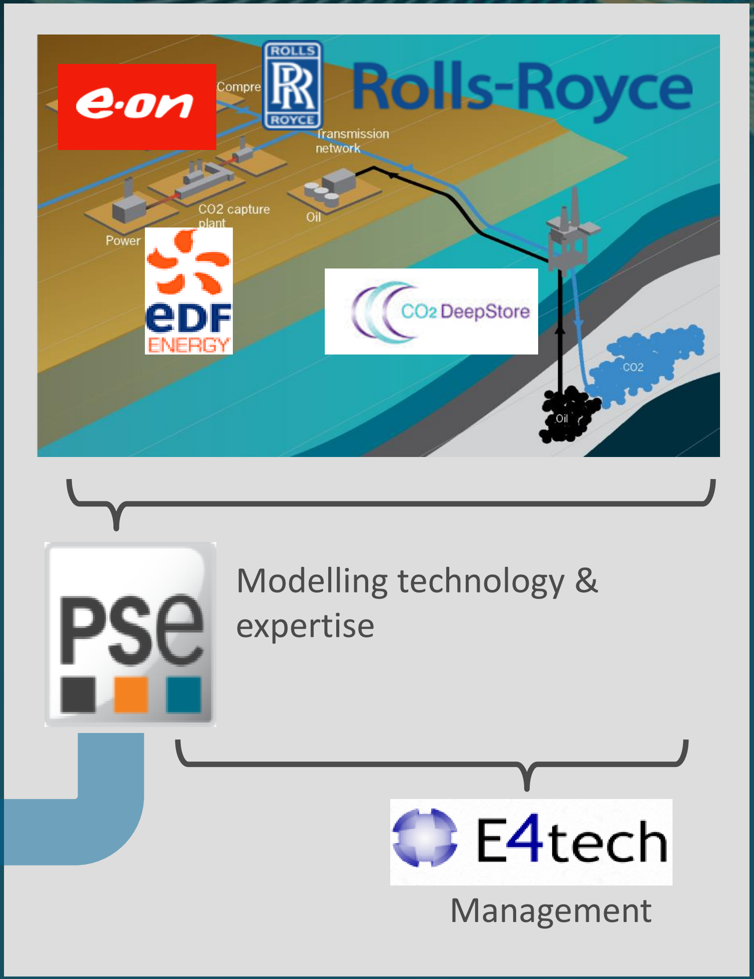
- Energy & Environment

CCS Advanced Process Modelling Tool-kit Project

- $5.5m project
- 3 year development (2011-2014)
- Tool tested using several case studies

energy technologies institute



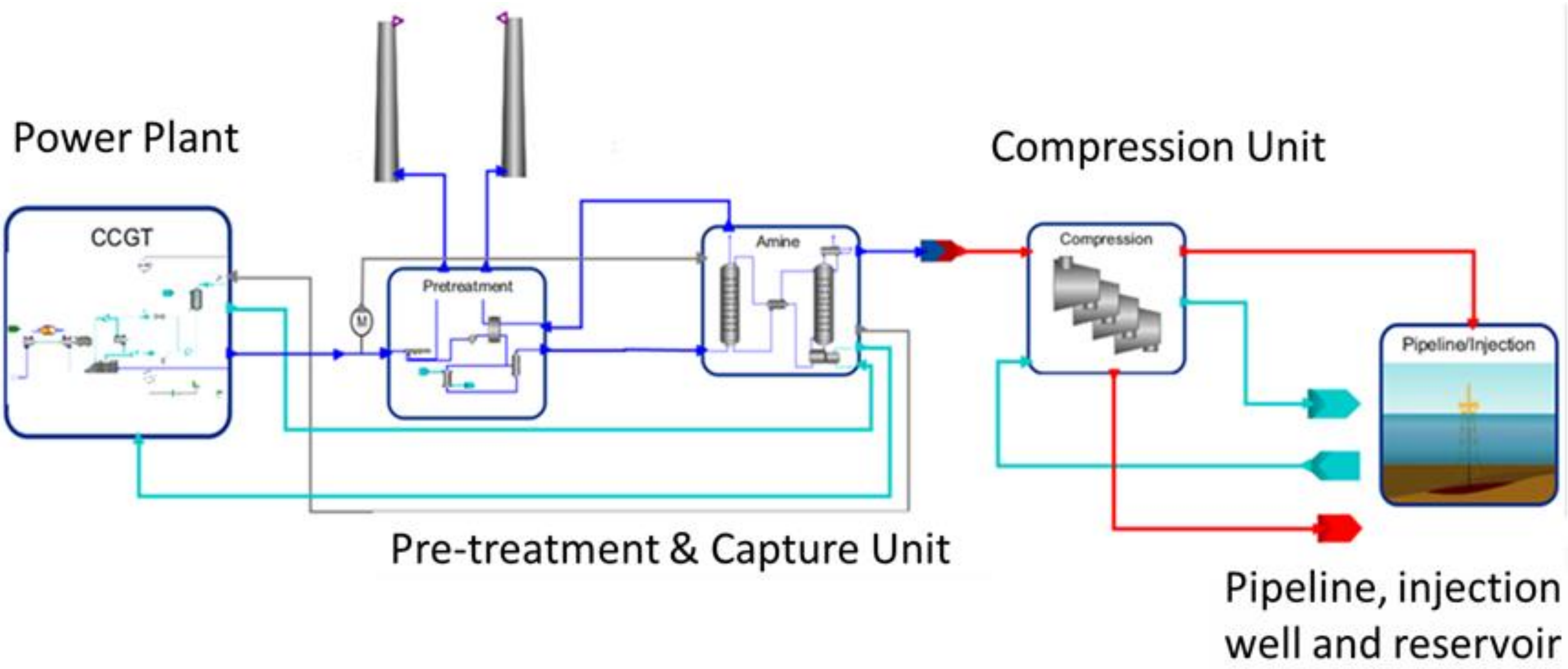


gCCS v1.1 scope

- **Process models**
  - Power generation
    - Conventional: PC, NGCC
    - Non-conventional: oxy-fuelled, IGCC
  - Solvent-based CO_2 capture
  - CO_2 compression & liquefaction
  - CO_2 transportation
  - CO_2 injection in sub-sea storage
  - CO_2 Enhanced Oil Recovery
- **Costing models**
  - Equipment CapEx & OpeX
- **Materials models**
  - cubic EoS (PR 78)
    - flue gas in power plant
  - Corresponding States Model
    - water/steam streams
  - SAFT-VR SW/ SAFT-γ Mie
    - solvent-containing streams in CO_2 capture
  - SAFT-γ Mie
    - near-pure post-capture CO_2 streams

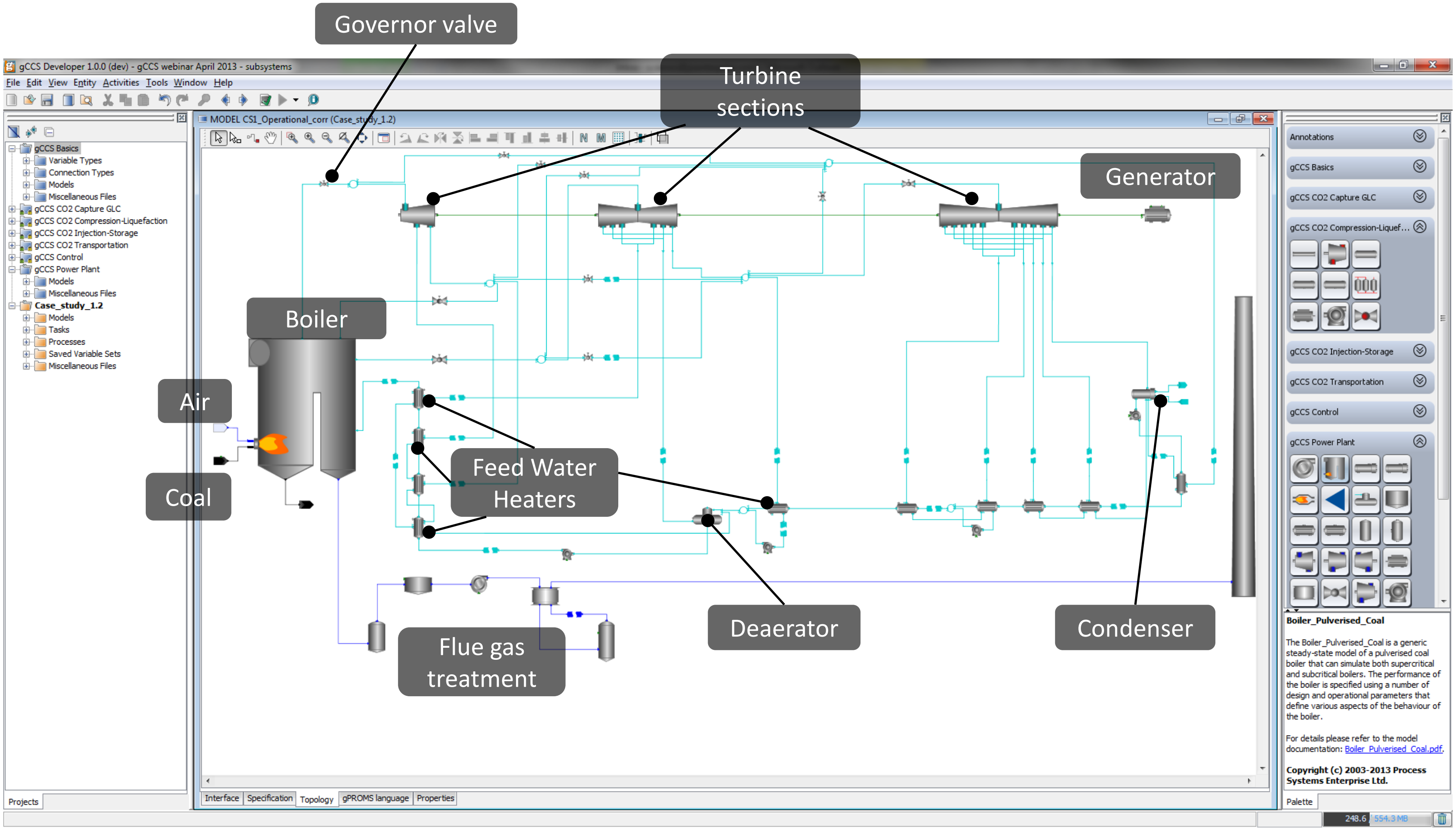
Open architecture allows incorporation of 3rd party models

Integrated CCS Chain flowsheet model

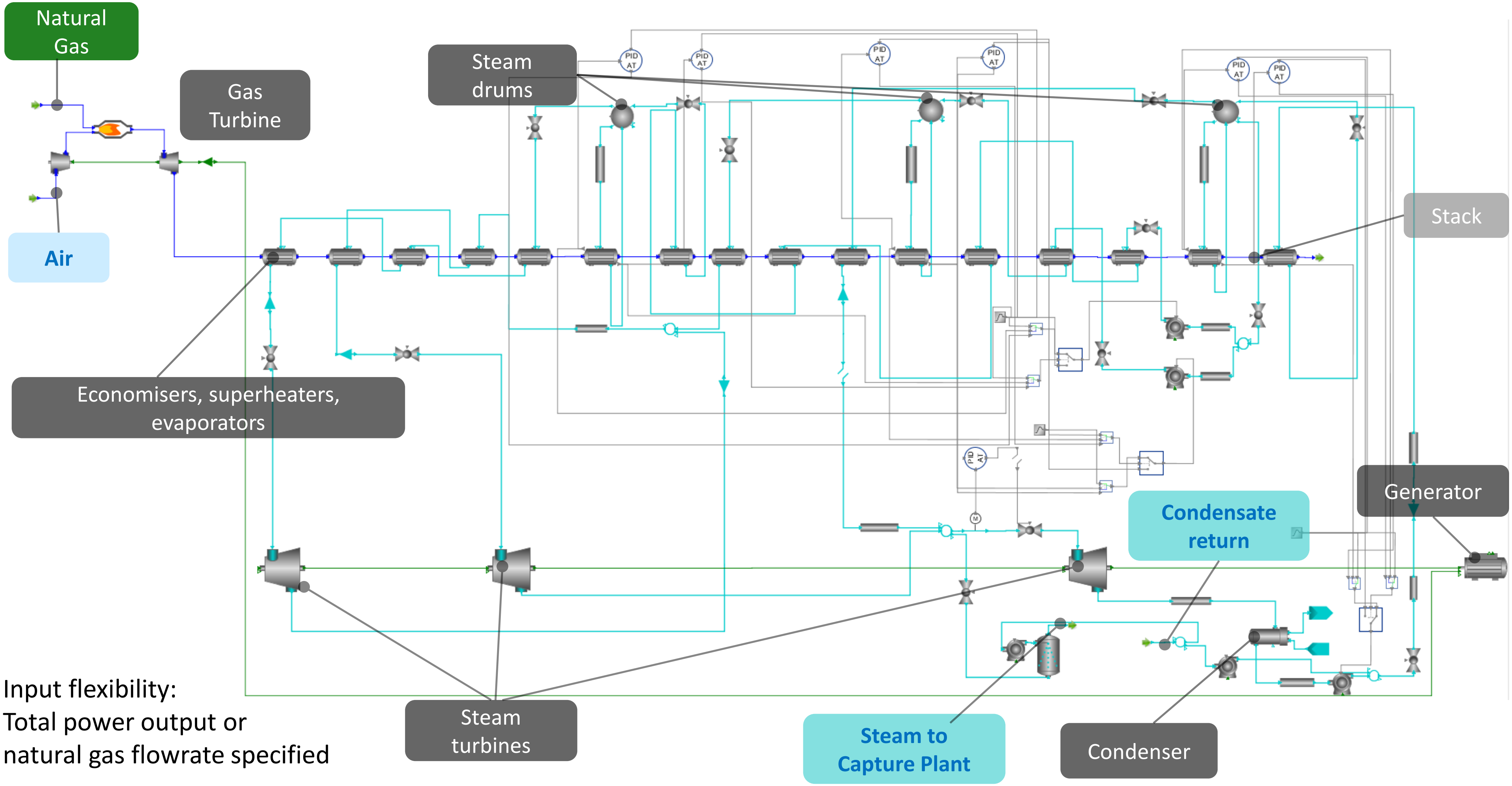


gCCS Power Plant library – conventional power generation

Supercritical pulverized coal power plant

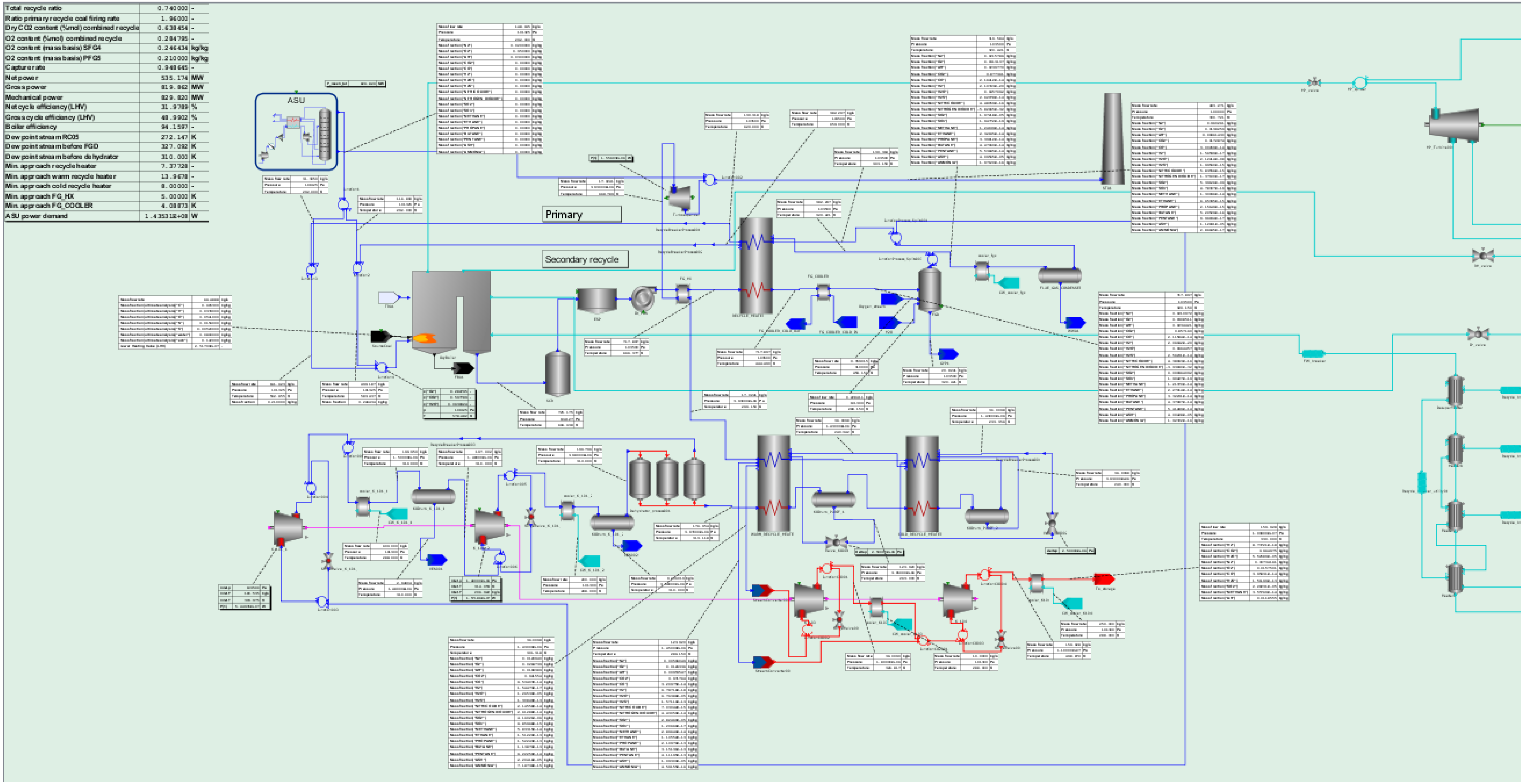


Combined Cycle Gas Turbine power plant



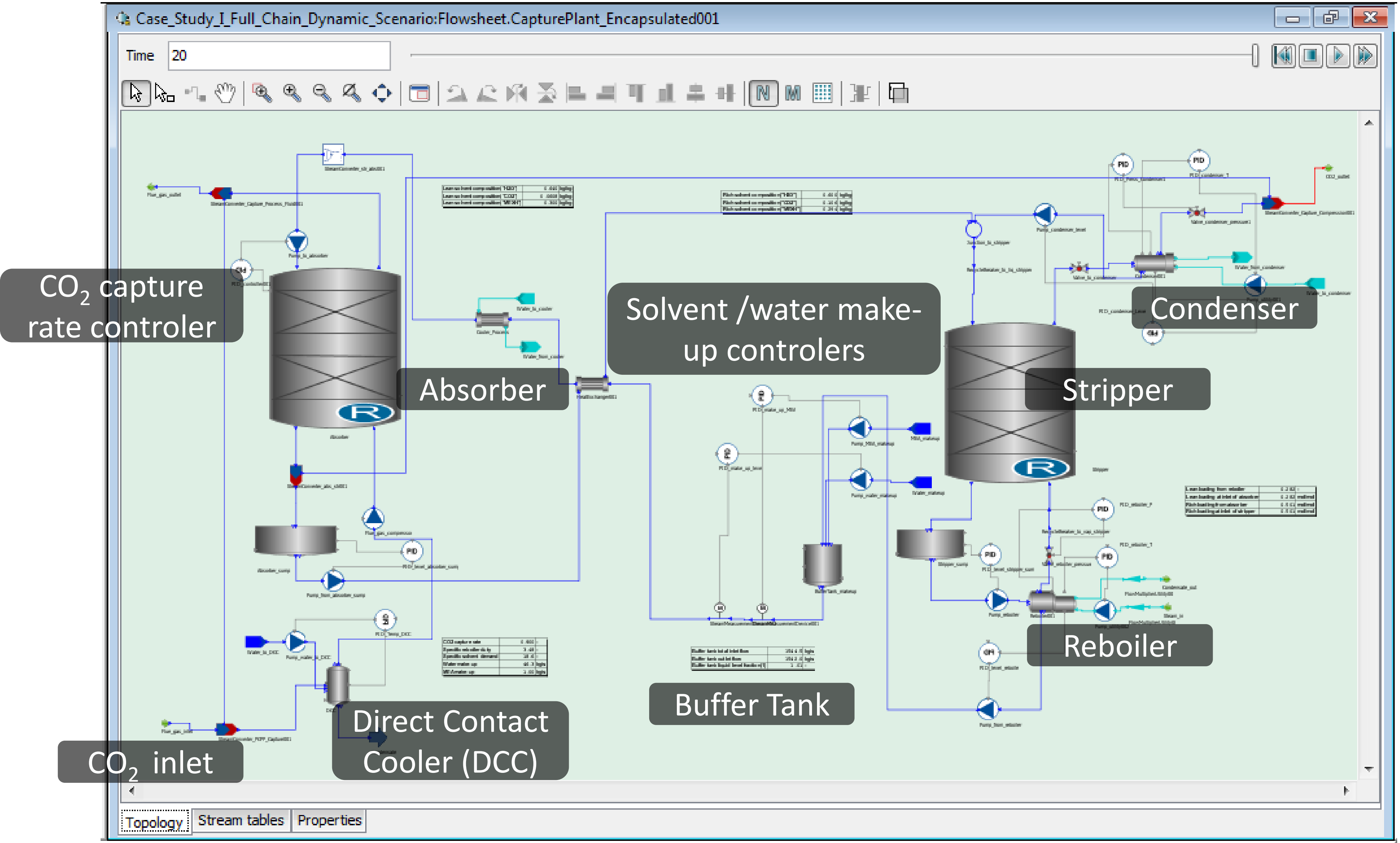
Input flexibility:
Total power output or natural gas flowrate specified

Oxyfuel system

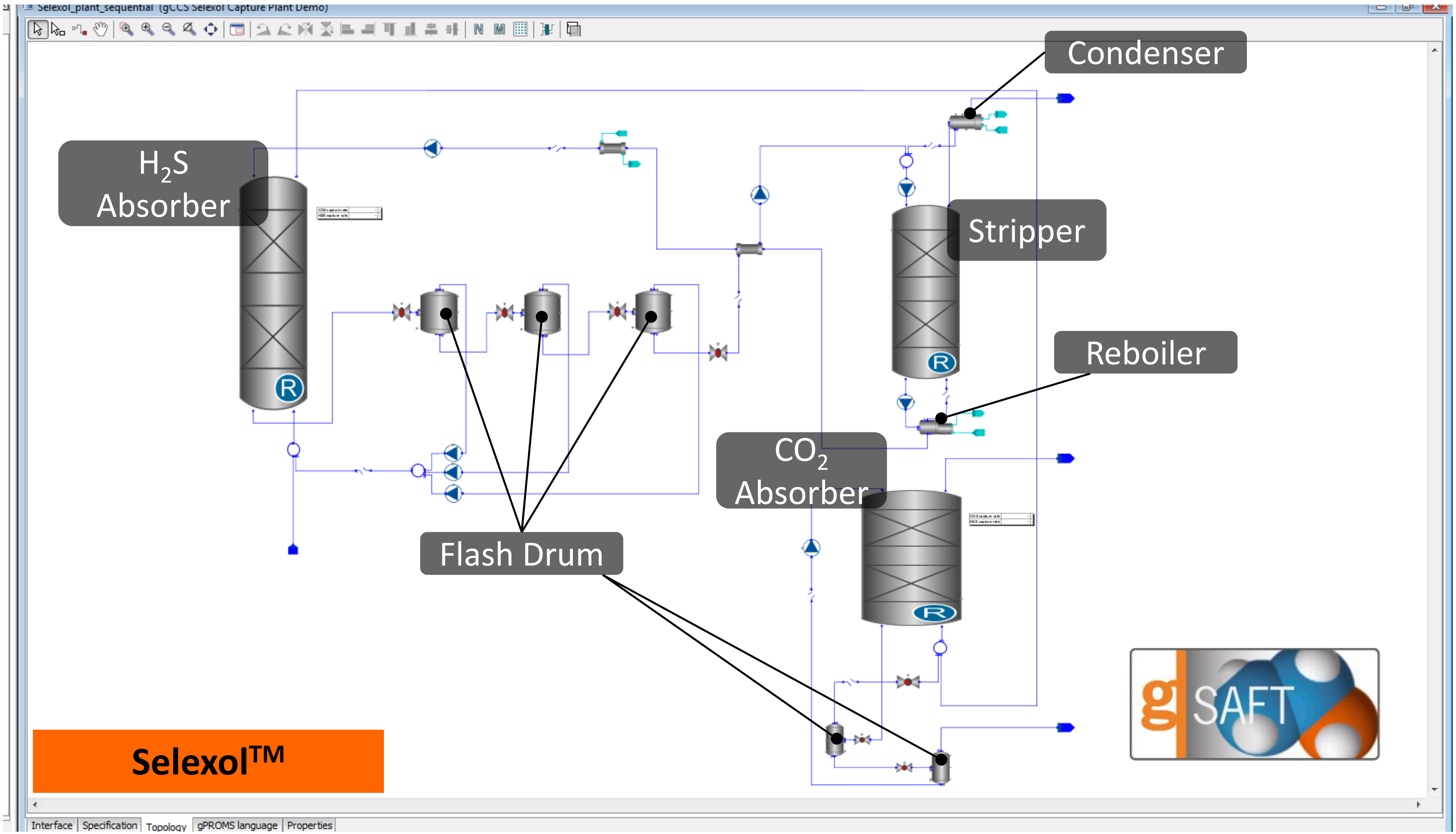


gCCS CO_2 Capture library – Solvent-based CO_2 capture

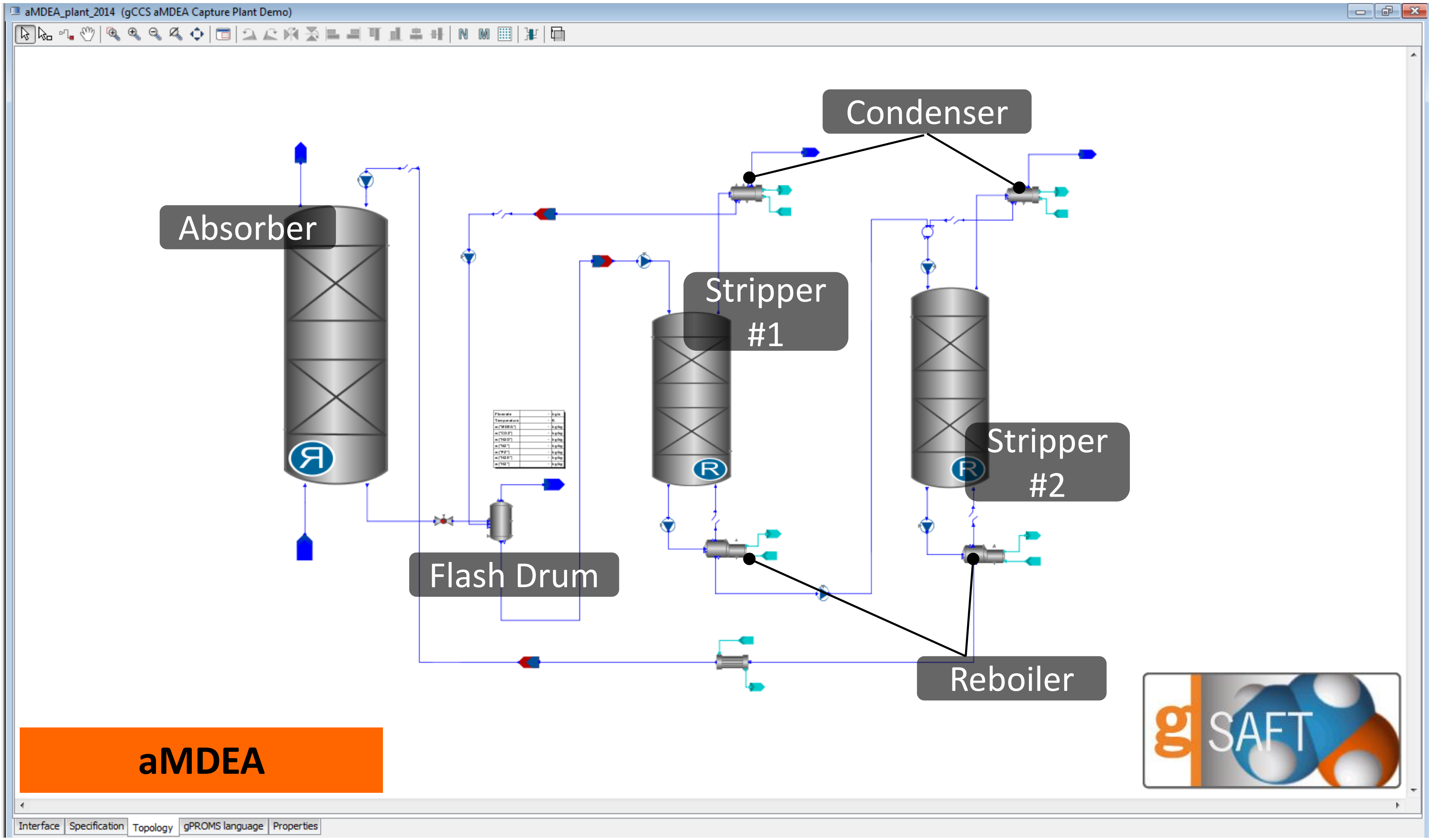
"Standard" Amine plant



Physical absorption (Selexol™ process)

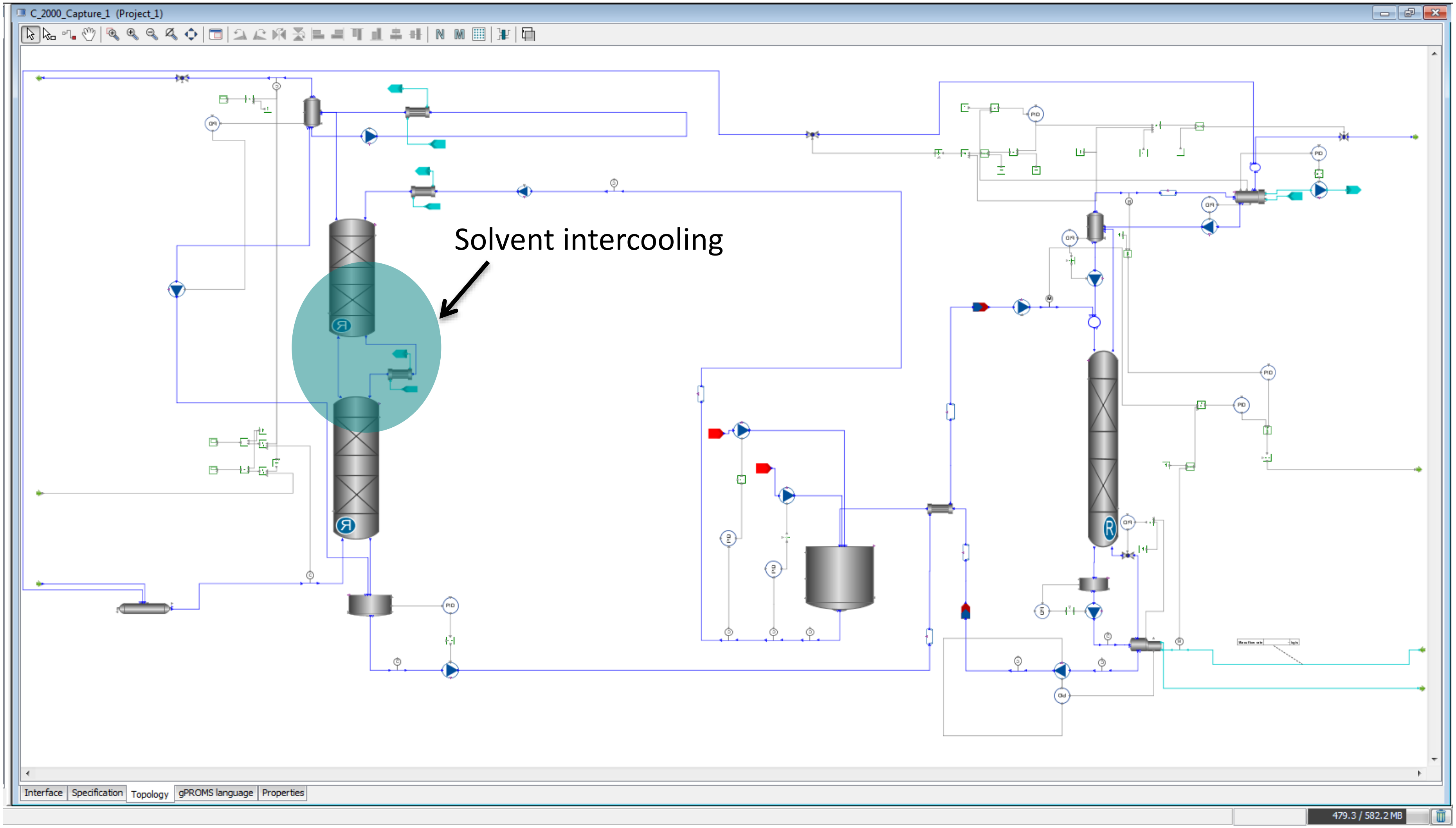


Activated amine capture plant



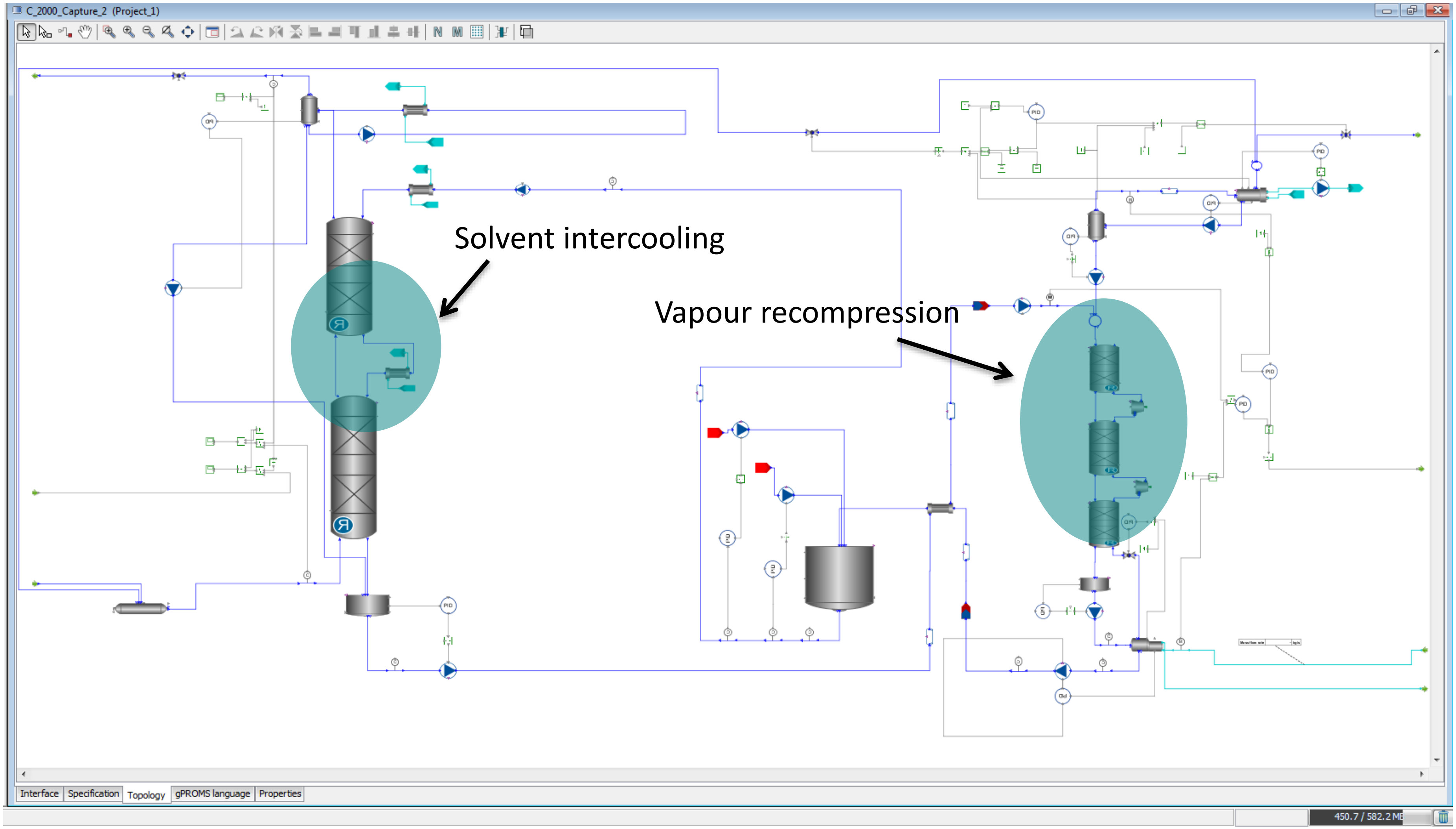
Advanced PCC configurations

- Alternative solvent-based capture plant

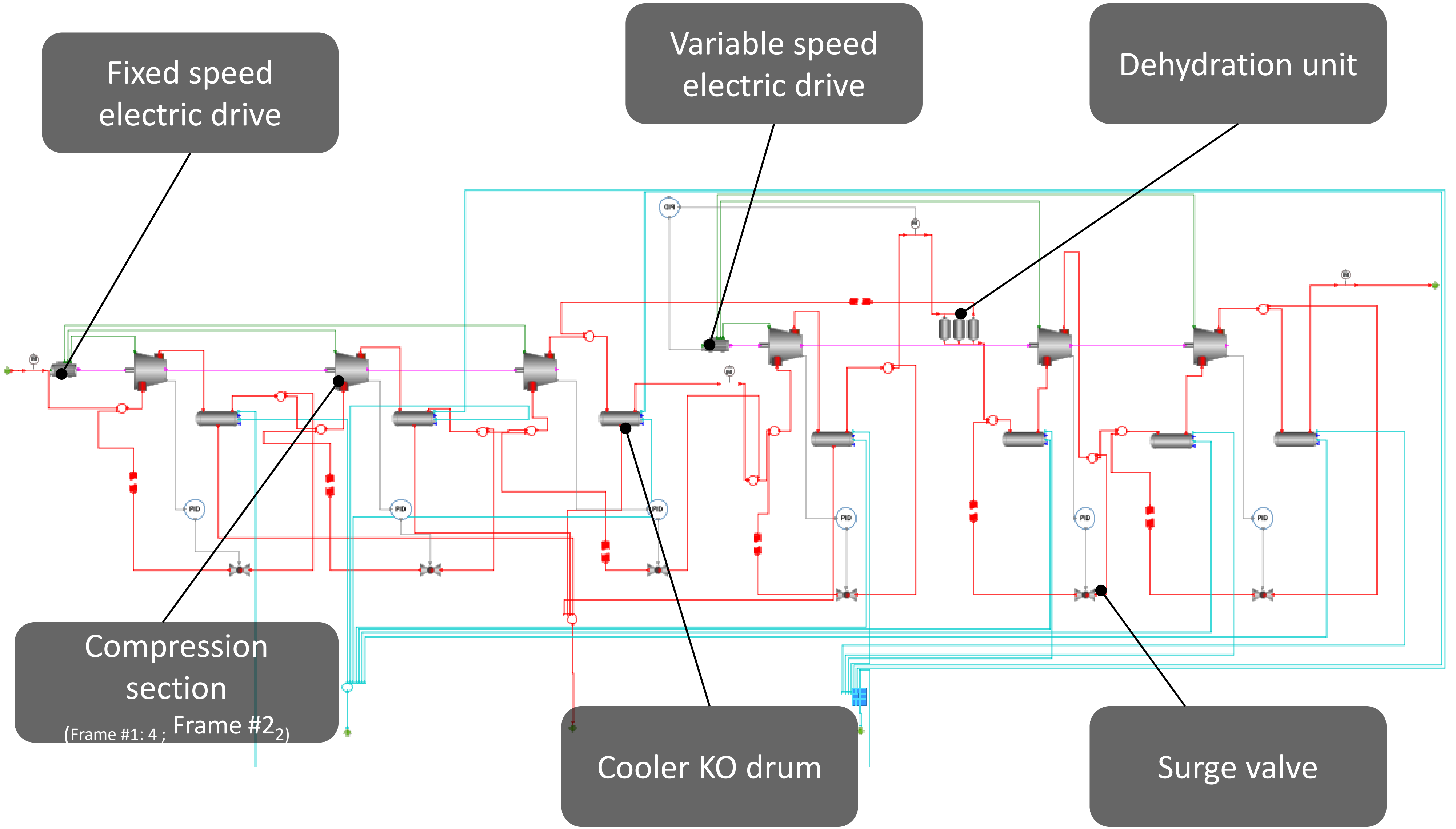


Advanced PCC configurations

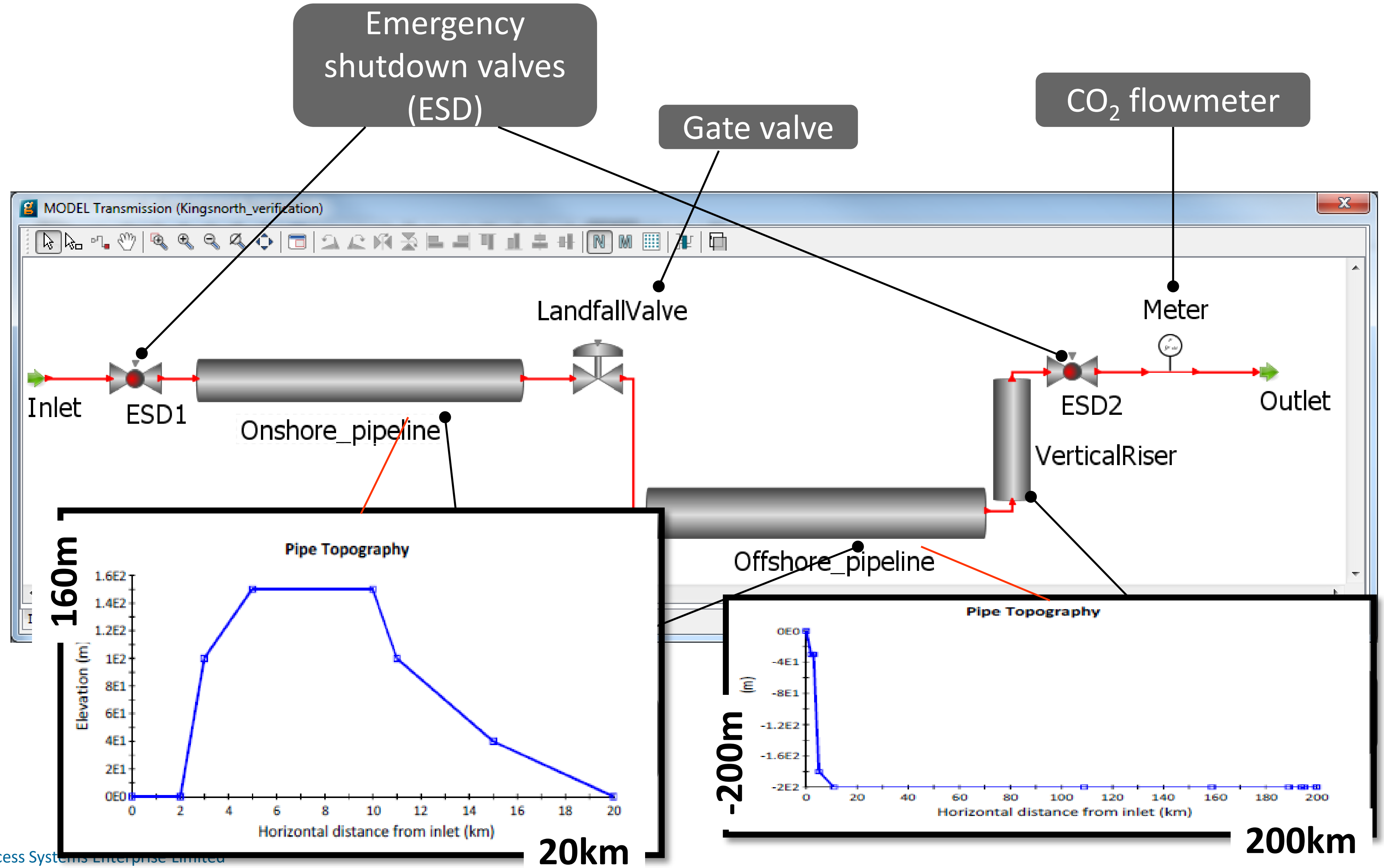
- Alternative solvent-based capture plant



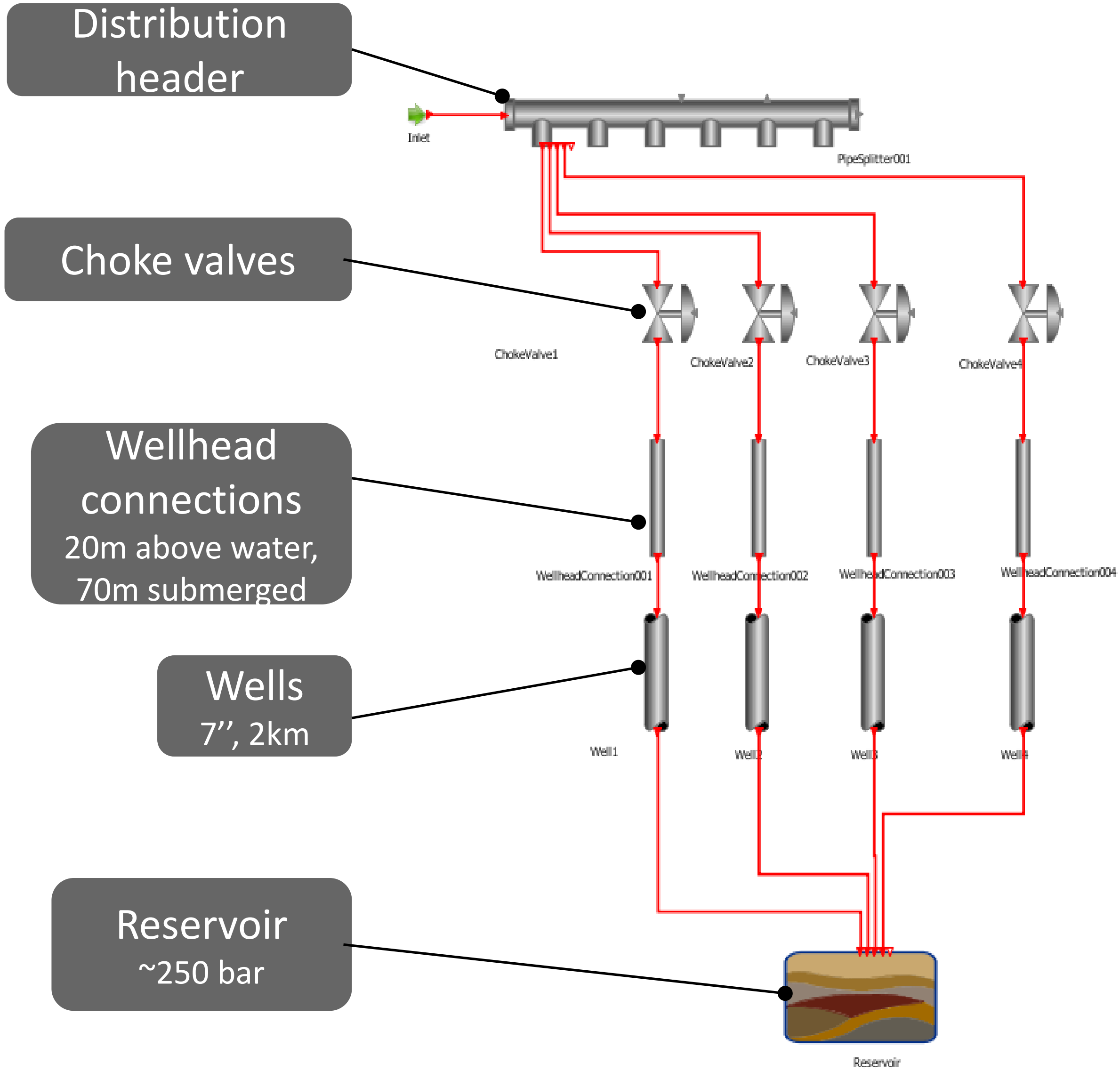
CO_2 compression plant



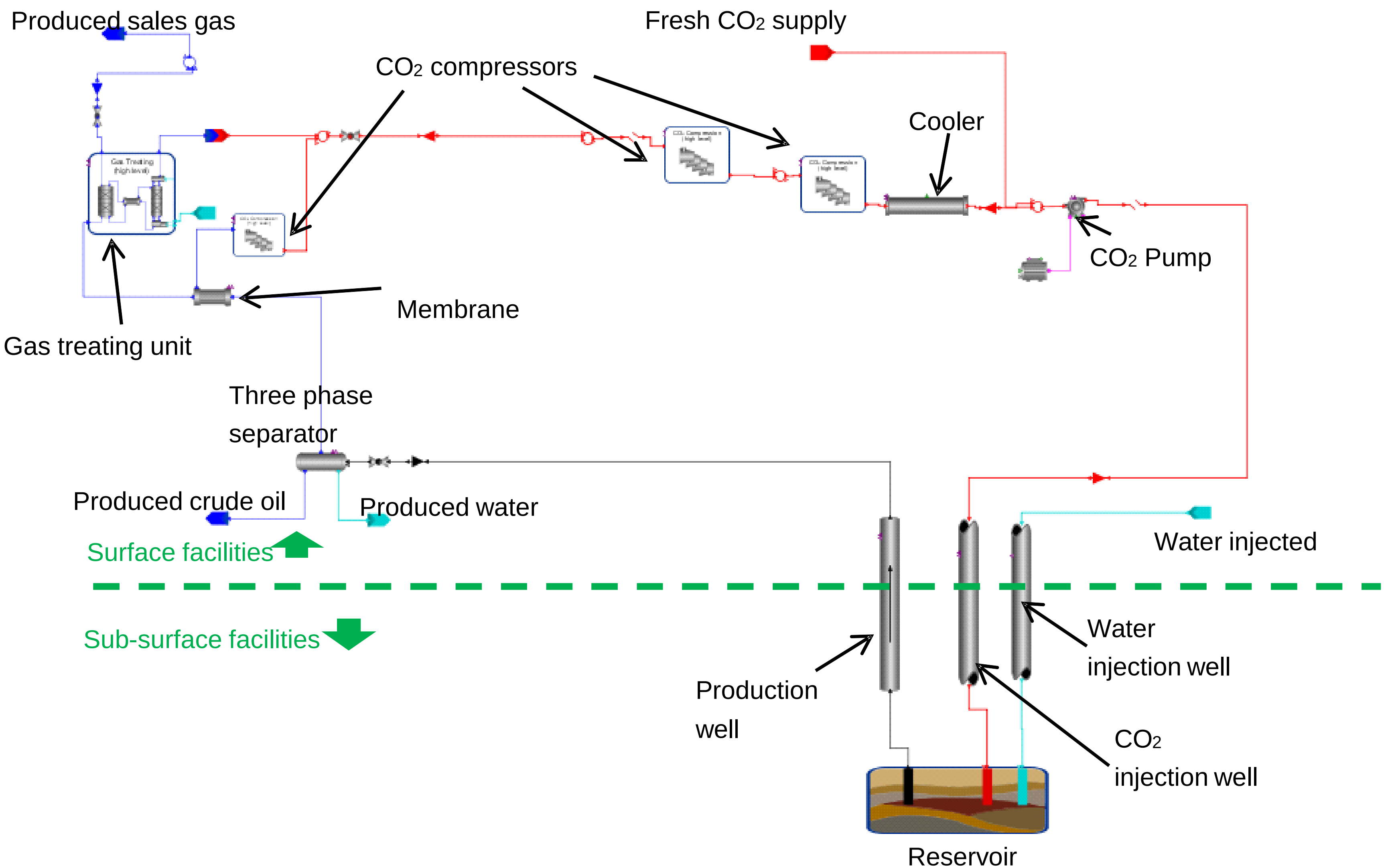
CO_2 transmission pipelines



CO_2 injection & storage in reservoir

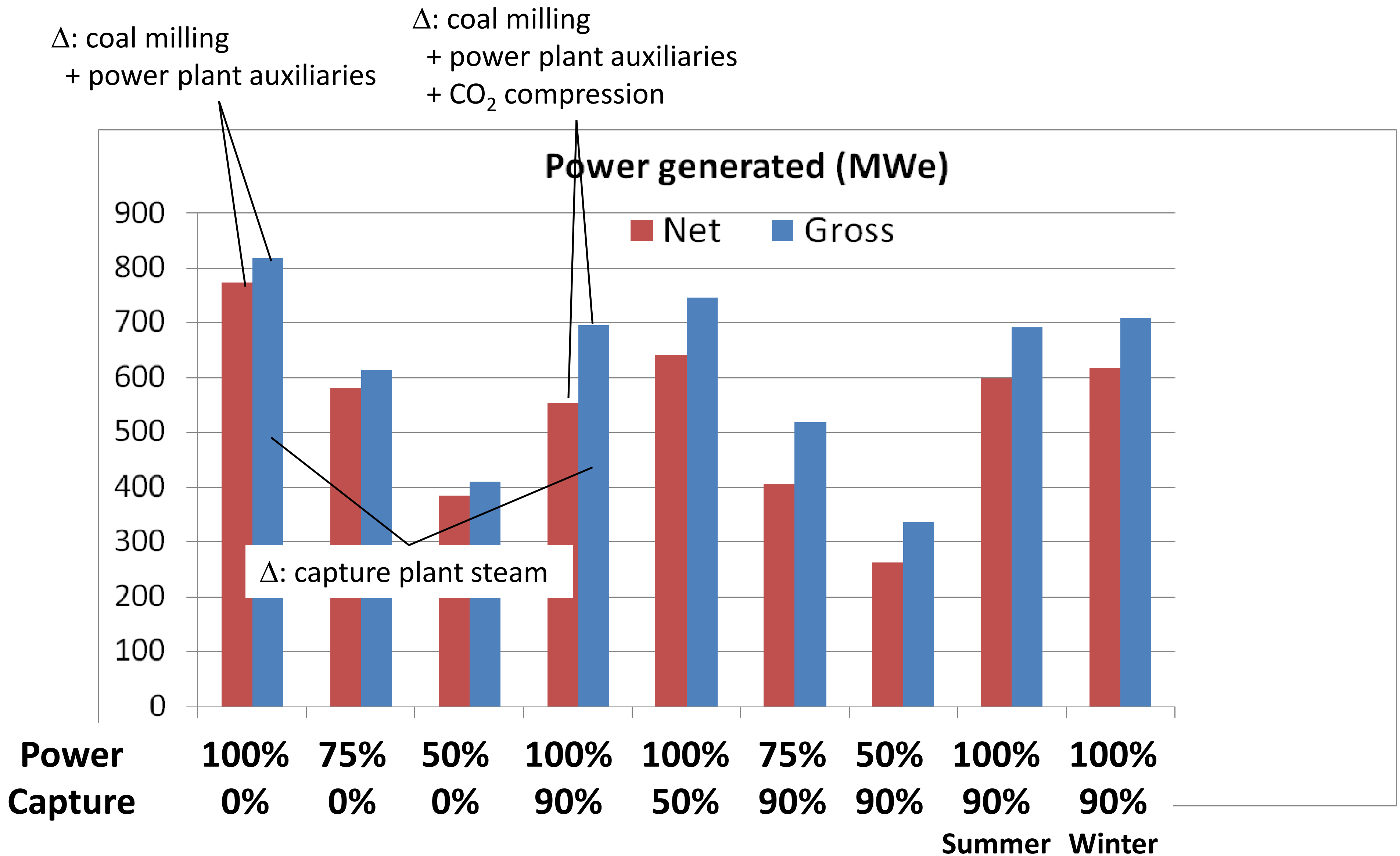


CO_2 EOR


Produced sales gas
Fresh CO2 supply
CO2 compressors
Cooler
CO2 Pump
Membrane
Gas treating unit
Three phase separator
Produced crude oil
Produced water
Surface facilities
Water injected
Sub-surface facilities
Water injection well
Production well
CO2 injection well
Reservoir

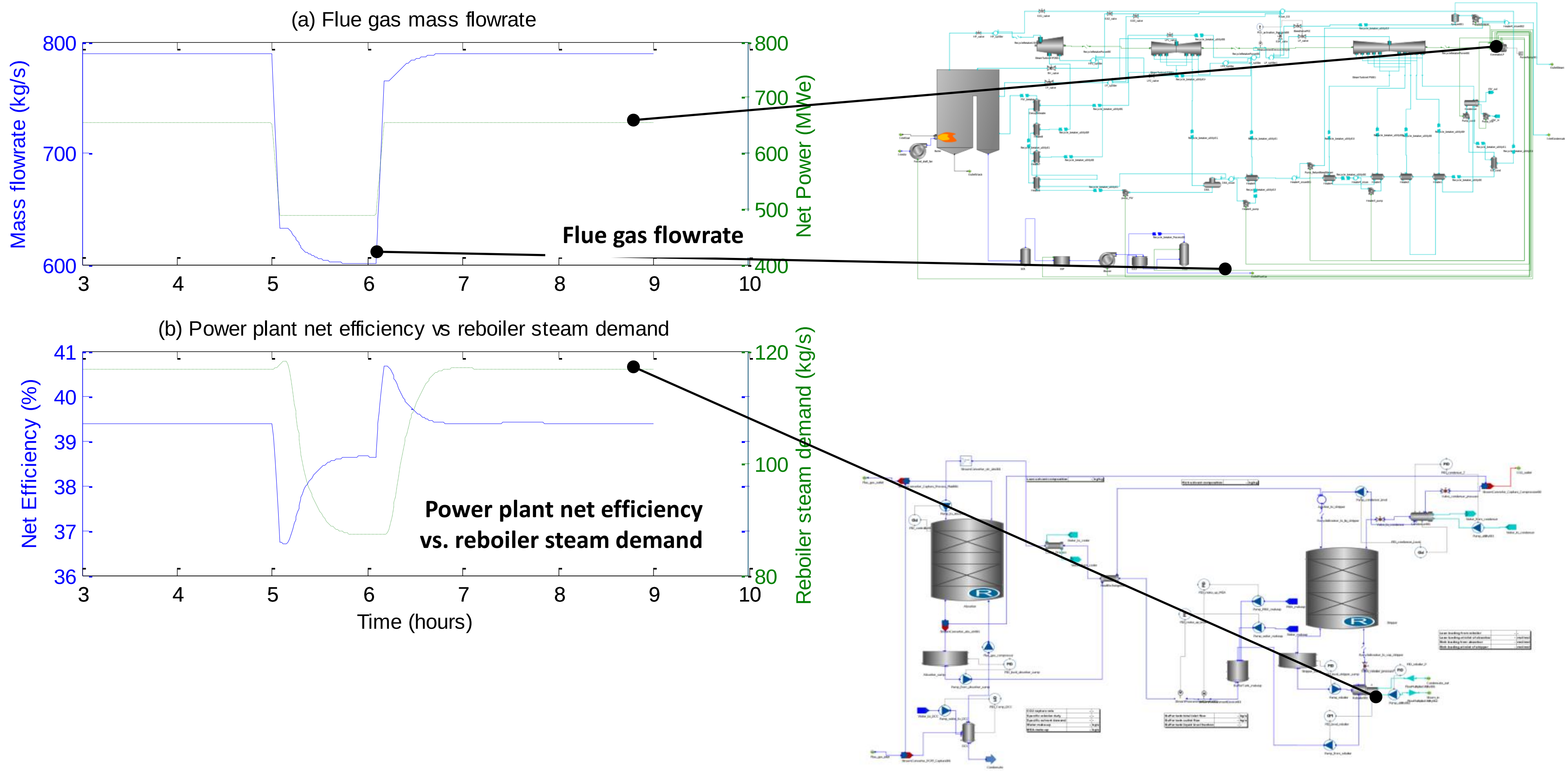
Steady-state analysis

Power generation



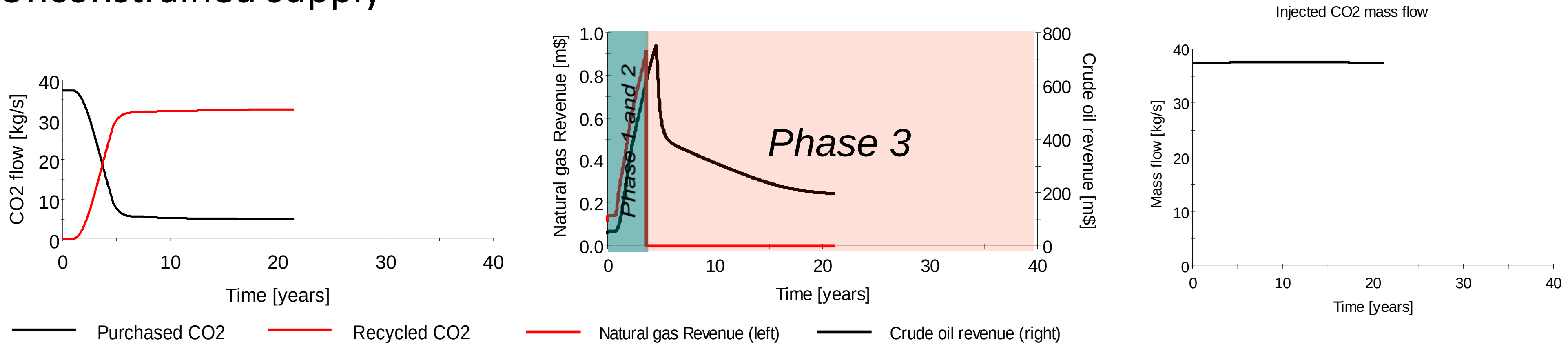
Operational analysis

Power/CO_2 capture two-way coupling

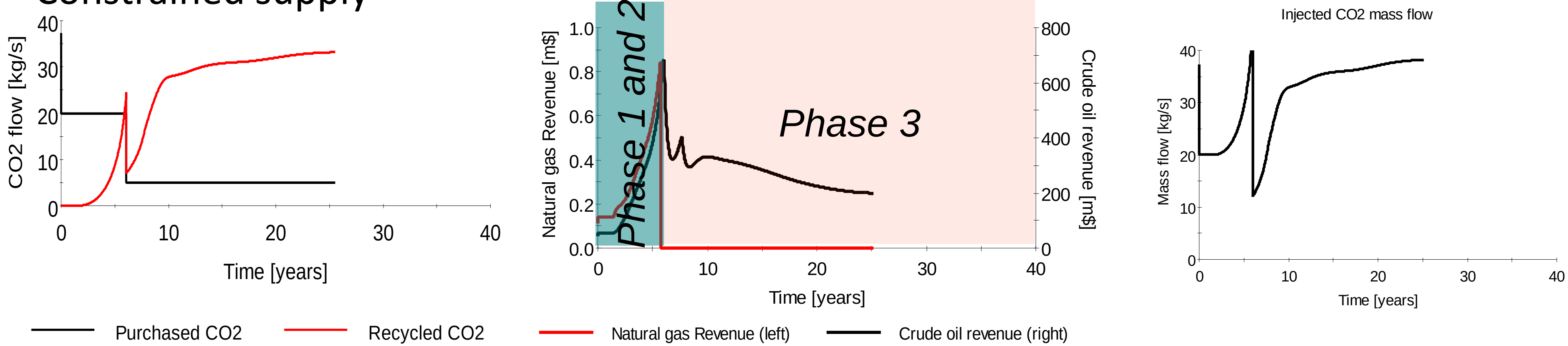


Analysis of CO_2 EOR with supply constraints

Unconstrained supply

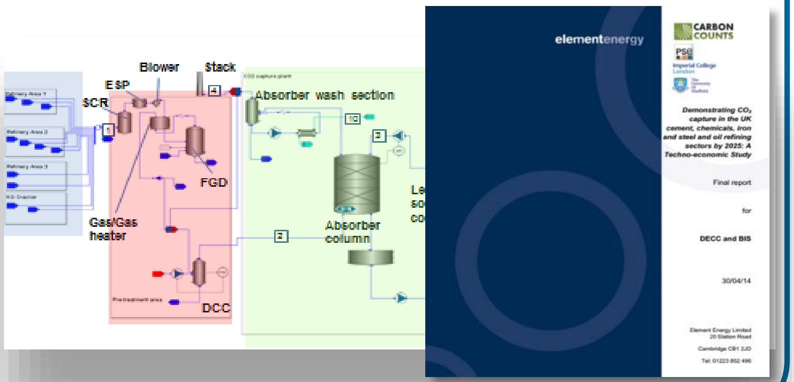


Constrained supply

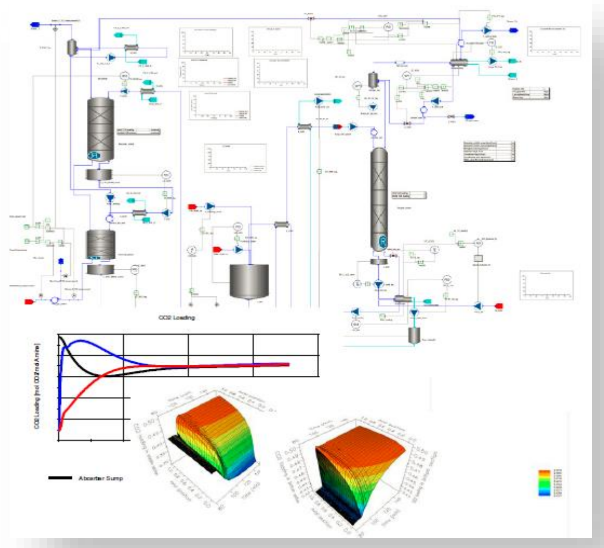


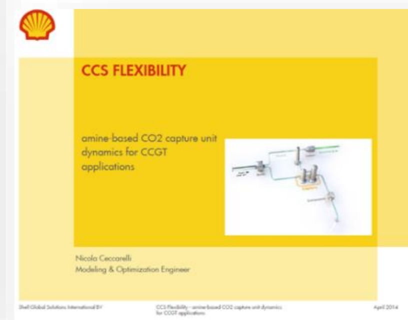
gCCS applications

Techno-economic study of Industrial Carbon Capture and storage [DECC and Element Energy]

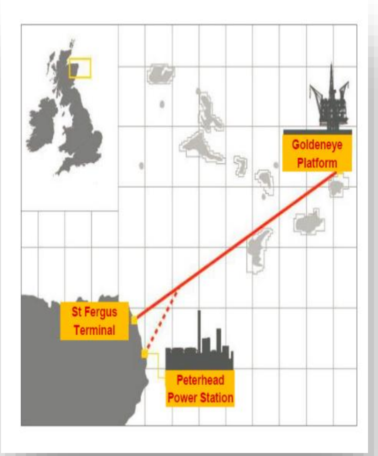


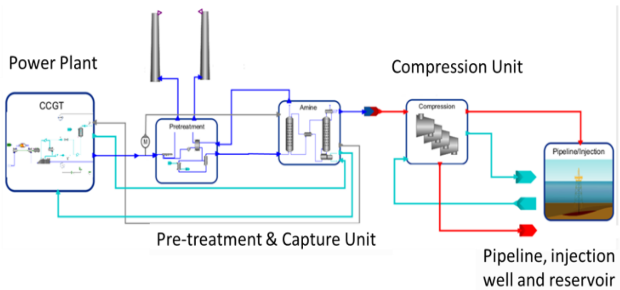
Optimizing start-up and shutdown procedures of gas treating plants [Shell]



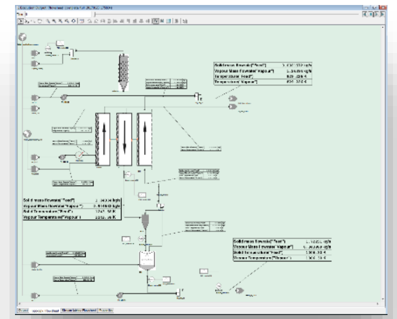


CCS chain and network studies [Energy Technologies Institute and Shell]





Development of novel technology for **L**ow **E**mission **I**ntensity **L**ime **a**nd **C**ement (LEILAC, Horizon 2020)



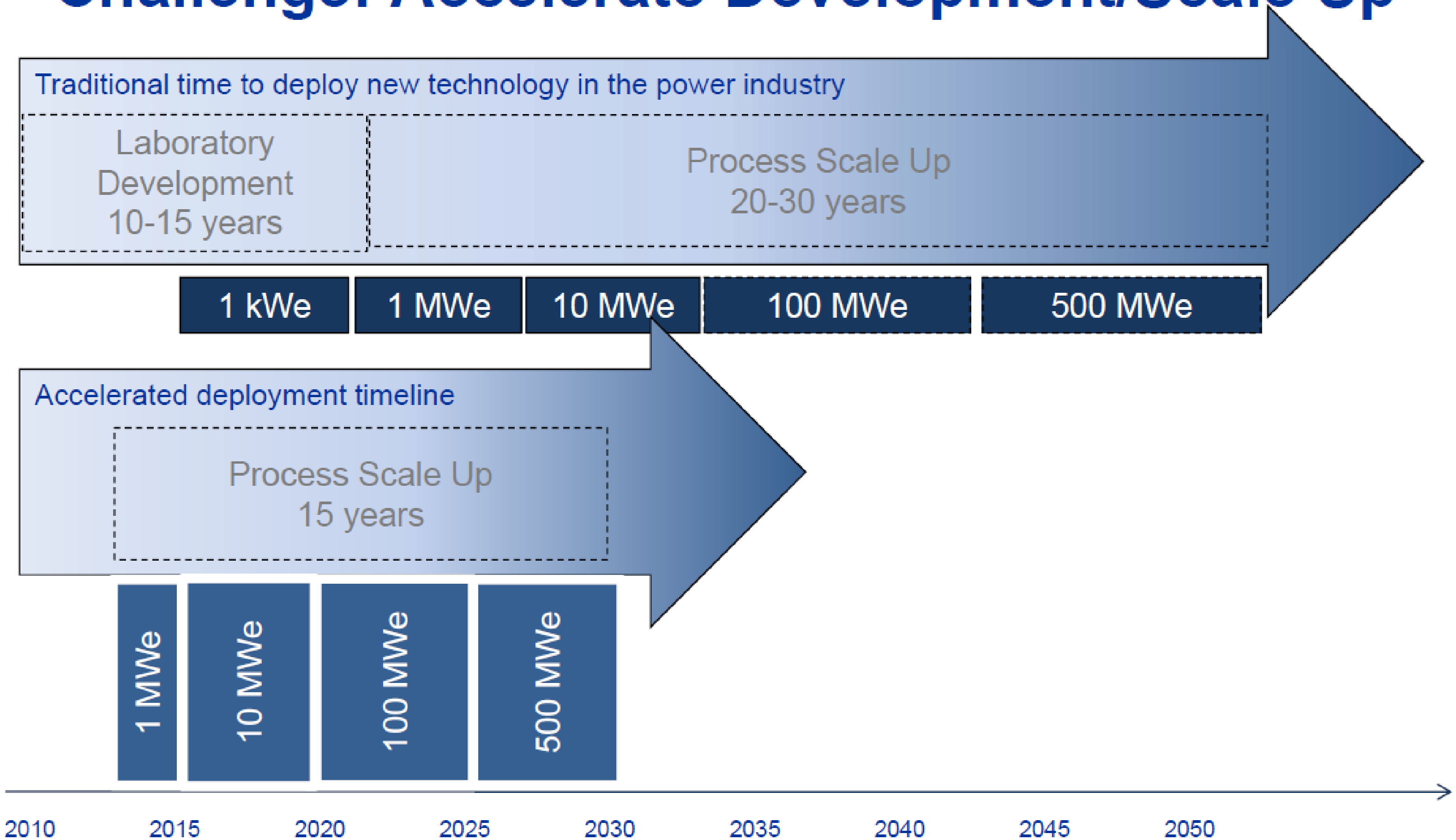
Leilac

The Carbon Capture Simulation Initiative (CCSI) commercialization project

Background

U.S. Carbon Capture Simulation Initiative (CCSI)

Challenge: Accelerate Development/Scale Up



CCSI Carbon Capture Simulation Initiative · NETL · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · Pacific Northwest National Laboratory · U.S. Department of Energy

David Miller (2016), CCSI[2] Overview and Key Capabilities, NETL CO2 Capture Technology Meeting

Carbon Capture Simulation Initiative (CCSI)

CCSI For Accelerating Technology Development

Carbon Capture Simulation Initiative

Rapidly synthesize optimized processes to identify promising concepts → Better understand internal behavior to reduce time for troubleshooting → Quantify sources and effects of uncertainty to guide testing & reach larger scales faster → Stabilize the cost during commercial deployment

National Labs

- Berkeley Lab
- Pacific Northwest National Laboratory
- NETL
- Los Alamos National Laboratory
- Lawrence Livermore National Laboratory

Academia

- Carnegie Mellon
- Princeton University
- West Virginia University
- Boston University
- The University of Texas at Austin

Industry

- ADA
- ALSTOM
- B&W
- GE
- EPRI Electric Power Research Institute
- FLUOR
- Phillips 66
- American Electric Power
- Southern California Edison
- Southern Company
- ExxonMobil
- Chevron
- URS
- Air Products
- Eastman
- aspentech
- ANSYS
- Schneider Electric
- PSE

Miller D C et al., (2015). Multi-scale modelling of carbon capture systems, IEAGHG, PCCC3

CCSI nominated for R&D 100 Awards

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100 Awards

August 3, 2016 - 8:14am

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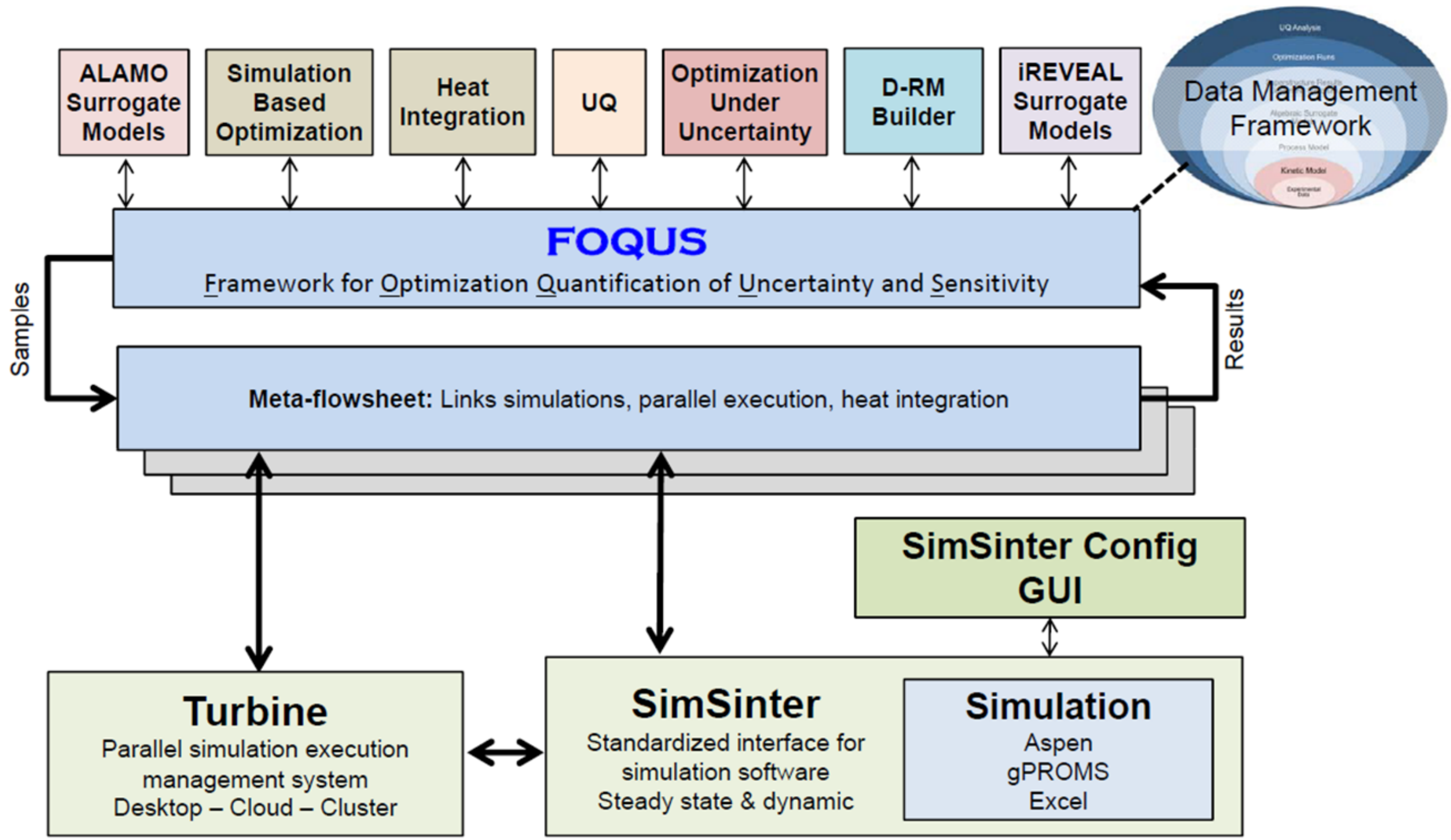
U.S. Carbon Capture Simulation Initiative (CCSI) Background



D. C. Miller, B. Ng, J. C. Eslick, C. Tong and Y. Chen, 2014, Advanced Computational Tools for Optimization and Uncertainty Quantification of Carbon Capture Processes. In *Proceedings of the 8th Foundations of Computer Aided Process Design Conference – FOCAPD 2014*. M. R. Eden, J. D. Siirola and G. P. Towler Elsevier.

Miller D C et al., (2015). Multi-scale modelling of carbon capture systems, IEAGHG, PCCC3

GE's CO_2 Solvent Separation Technology

Features

- Non-aqueous aminosilicone solvent, low water usage, low corrosivity
- Smaller footprint, simpler design, lower capital cost, lower operating cost
- Mature unit operations, robust system integration & heat management
- Low volatility (emissions),
- Successful bench scale demo completed

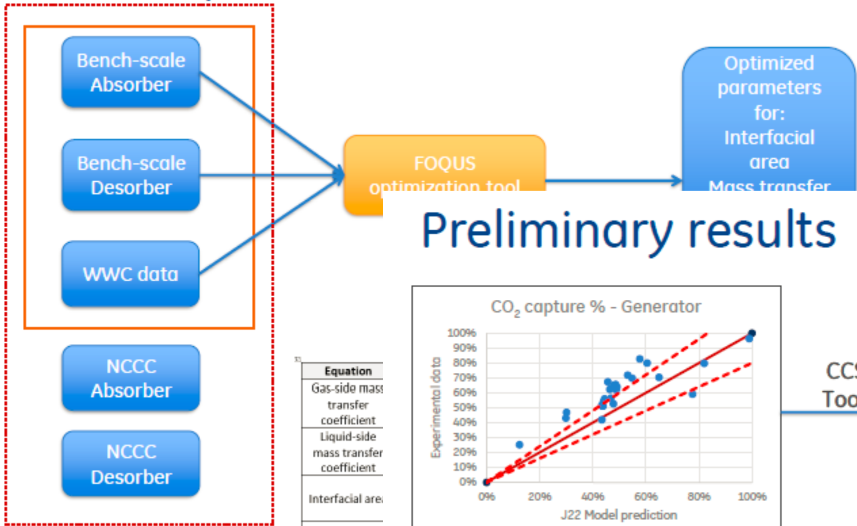
imagination at work

Bench scale CO_2 Capture Skid

Small Scale Pilot (0.5MW)

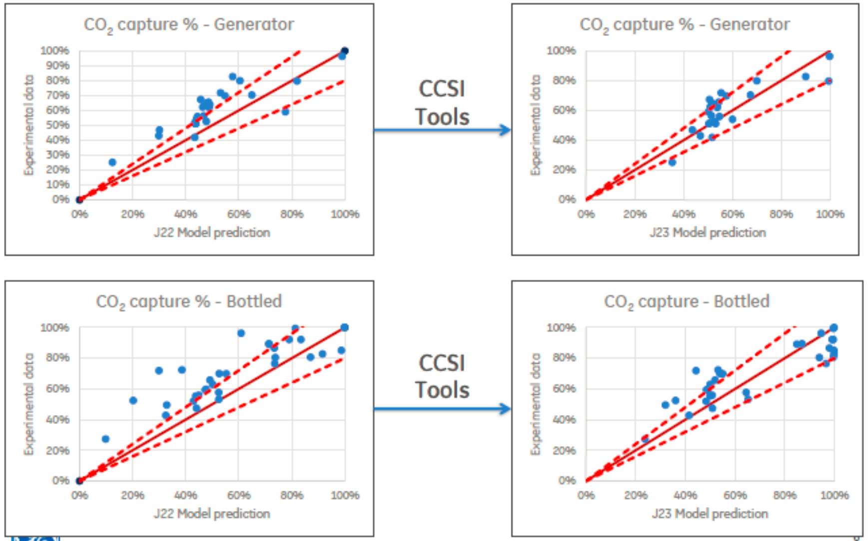
- Scope: Design, construct & test a pilot scale facility at the National Carbon

FOQUS Optimization



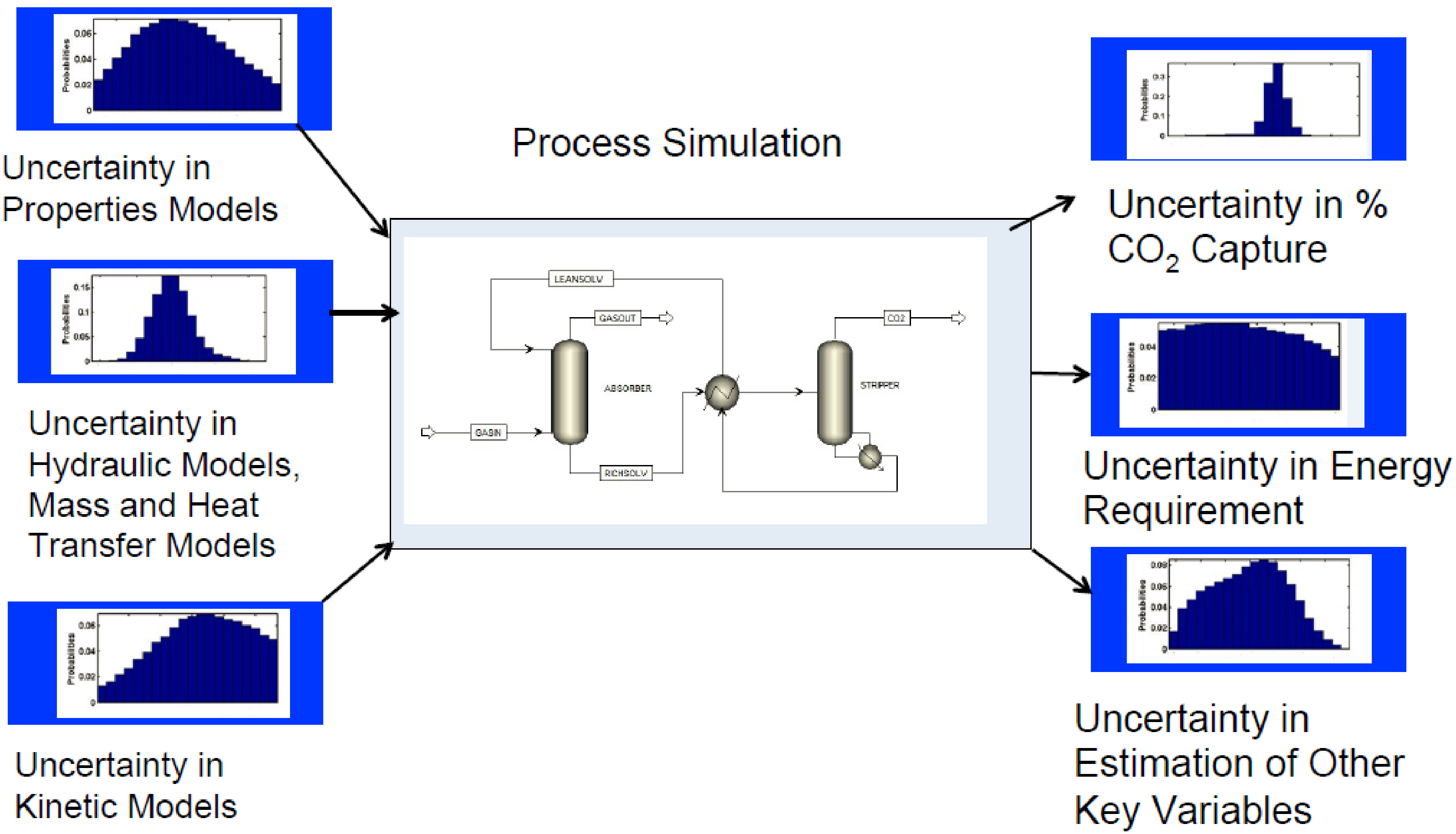
Equation
Gas-side mass transfer coefficient
Liquid-side mass transfer coefficient
Interfacial area
Reaction rate

Preliminary results



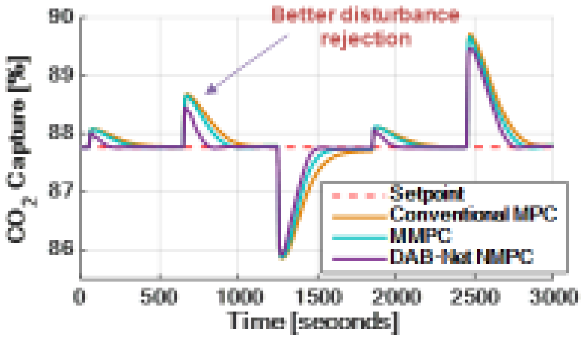
Teresa Grocela-Rocha (2016). Industrial Success Story: DOE-GE CRADA for CCSI Modeling, NETL CO2 Capture Technology Meeting

Uncertainty quantification in solvent systems



Morgan, J. C., D. Bhattacharyya, C. Tong and D. C. Miller (2015). "Uncertainty Quantification of Property Models: Methodology and Its Application to CO2-Loaded Aqueous MEA Solutions1." AIChE Journal. DOI: 10.1002/aic.14762

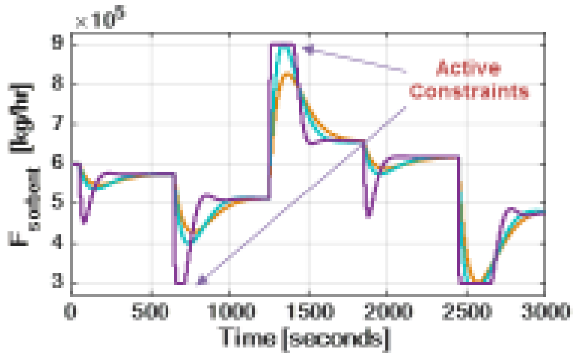
Performance Comparison on 2-Stage BFB Adsorber (ACM)

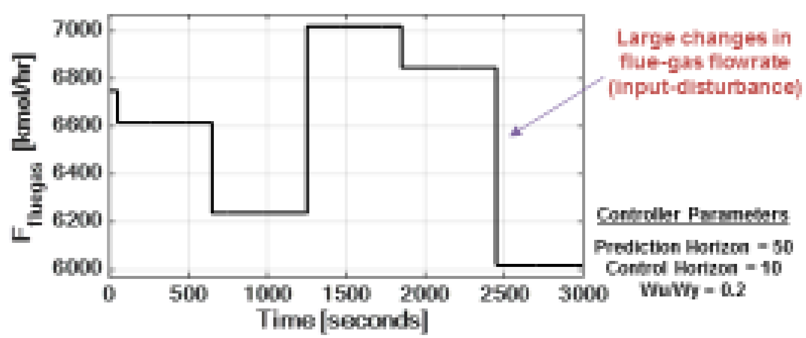


Controller responses to drastic plant-load changes – Comparison with standard MPC controller

Algorithm	Cumulative Residual	Computational Cost		
		Cumulative Control Calculation Time (sec)	Max Control Calculation Time (sec)	Total Simulation Time (min)
Conventional MPC	0.019	9.54	0.33	18.39
MMPC	0.016	10.14	0.41	18.43
DAB-Net NMPC	0.007	19.97	3.43	18.92

Note: Max. Control Calculation Time << Sample Time (T_s = 20 sec), Real-Time Operation with APC





11

Priyadarshi Mahapatra, Stephen E. Zitney (2016) APC Framework

The Carbon Capture Simulation Initiative (CCSI) commercialization project

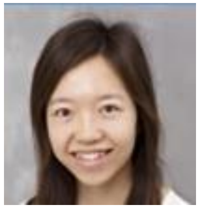
Project overview

Project partners ...and team

Principal Investigator (Technical)

Principal AE

AE - ALAMO



AE - SorbentFit

US Team

Co-Principal Investigator (Commercial)

Project Manager

Consultant

UK Team

WestVirginiaUniversity

Prof Debangsu Bhattacharyya
Co-Principal
Task leader Process Modelling

Researcher student
- Anca Ostace

Prof David Mebane
Co-Principal
Task leader Sorbentfit/SolventFit

Researcher students
- Keenan Kocan
- Alejandro Mejia

Carnegie Mellon University, Pittsburgh Pennsylvania 1900

Prof Nick Sahinidis
Co-Principal
Task leader ALAMO/FOQUS

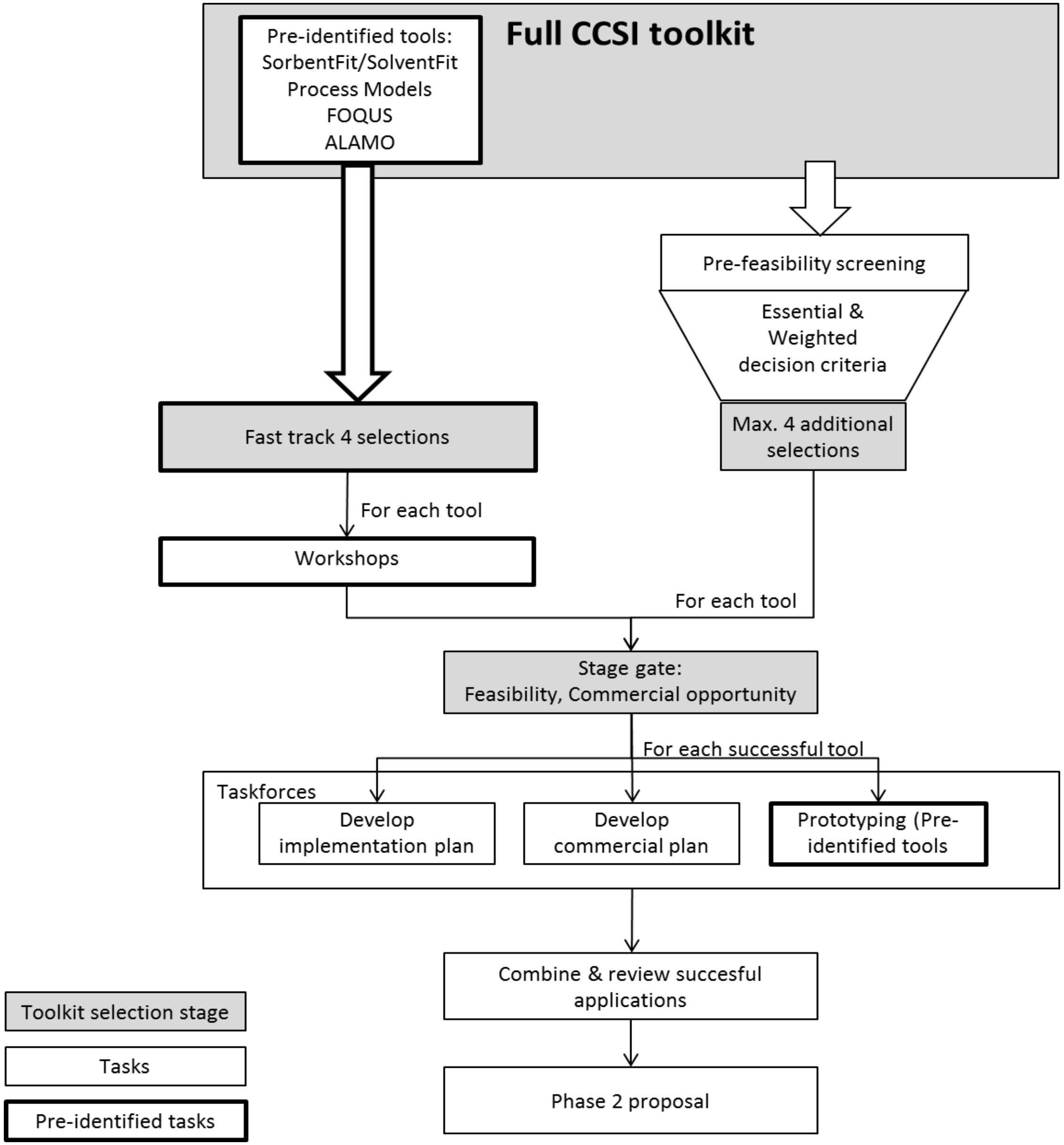
Researcher fellow
- Dr Mustafa Kilinc

Project objectives

- Identify opportunities for commercialising components of the CCSI toolkit within the gPROMS platform
  - Assessment and ranking of tools according to commercial and technical criteria

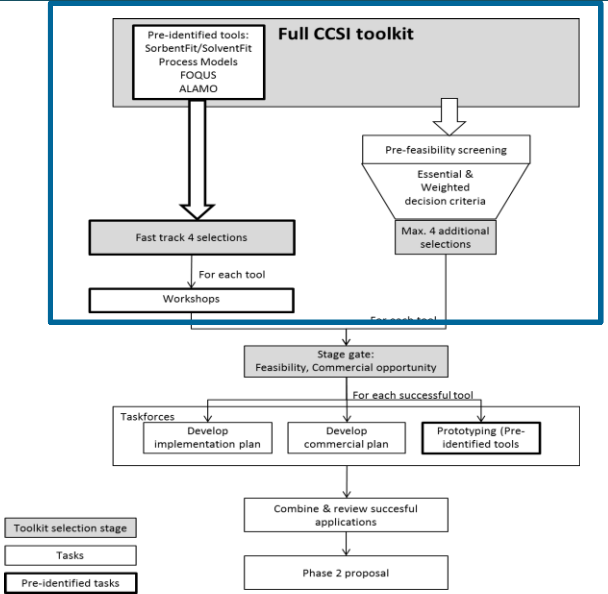
- Develop and demonstrate a clear technical delivery path towards achieving these opportunities
  - Devise implementation plans and build team for Phase 2

Project overview

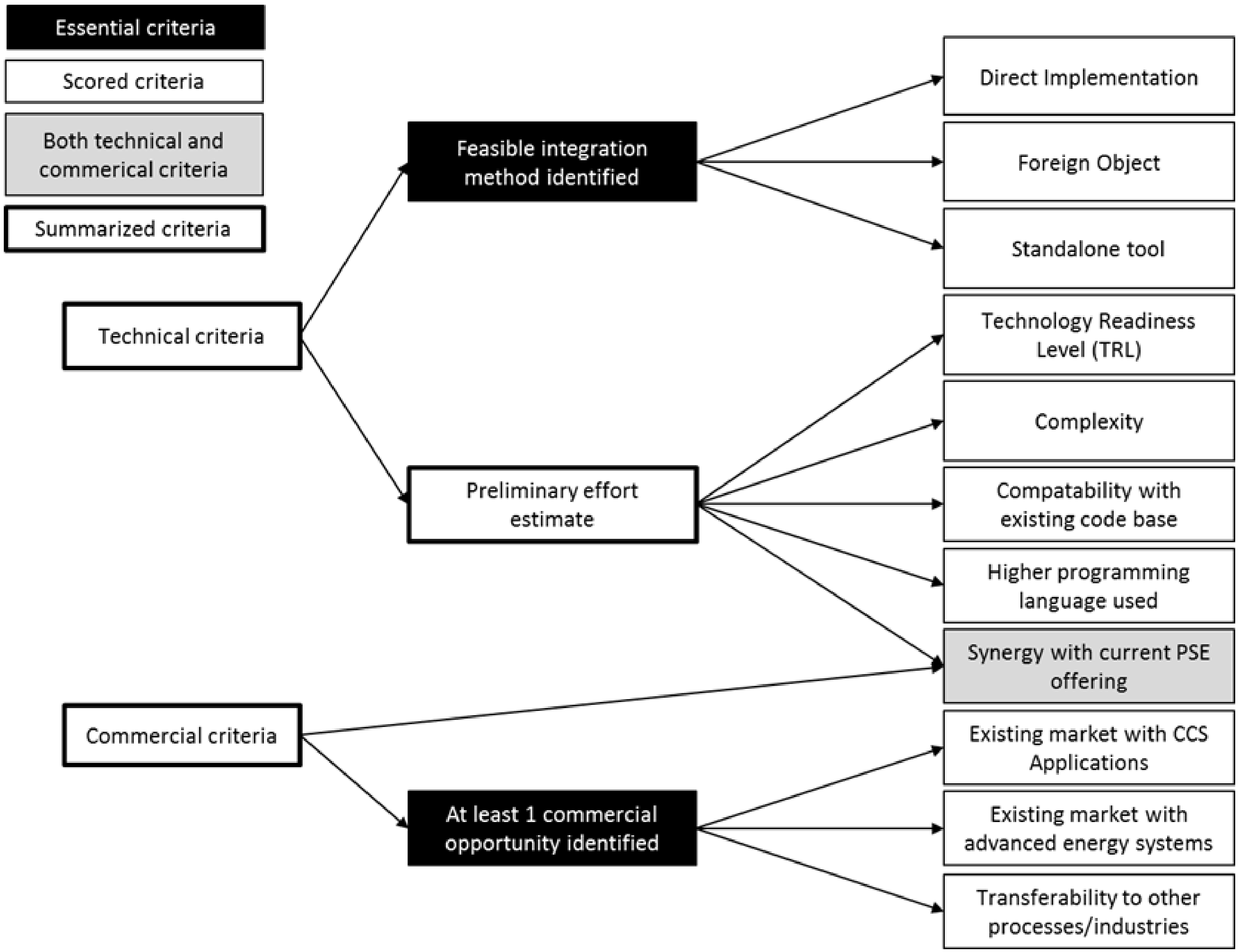


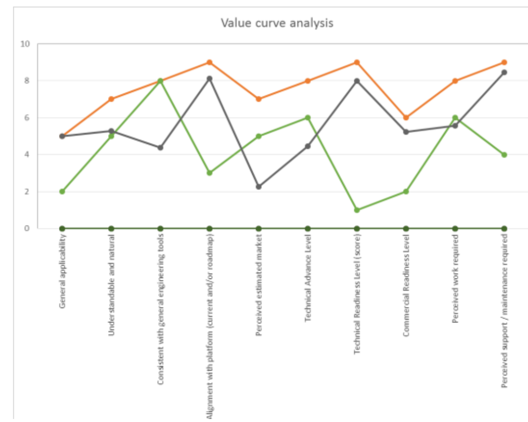
The Carbon Capture Simulation Initiative (CCSI) commercialization project

Screening and assessments



Proposed screening criteria

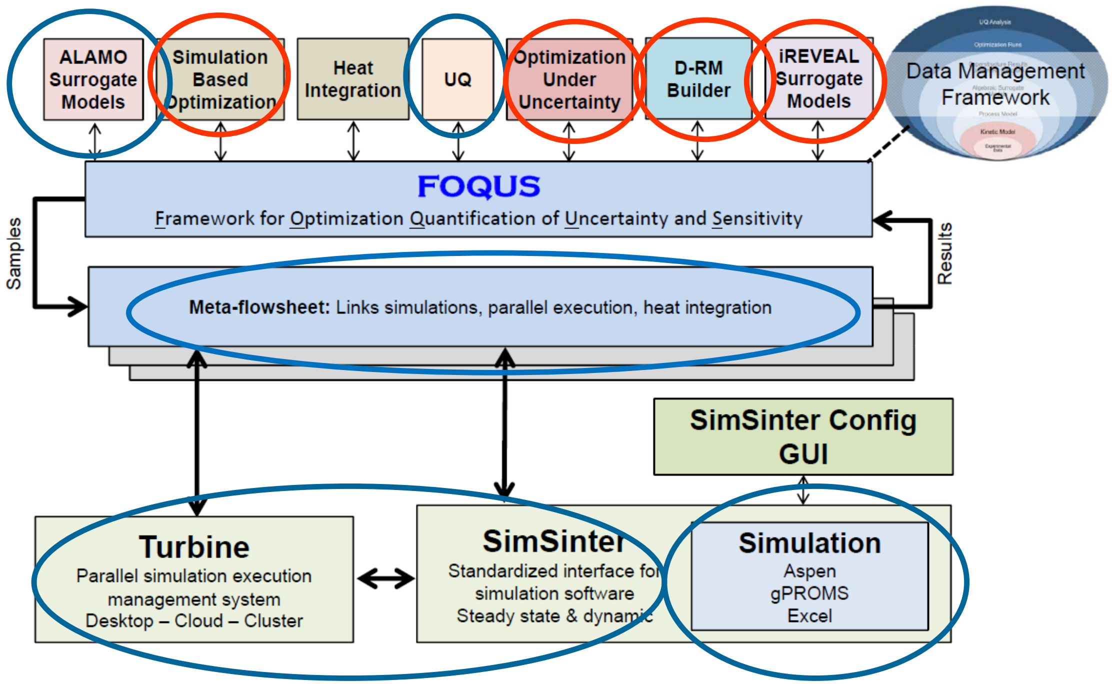




Carbon Capture Simulation Initiative (CCSI)
Fast track tools and screened tools

ALAMO

SolventFit/SorbentFit



Fast track tools

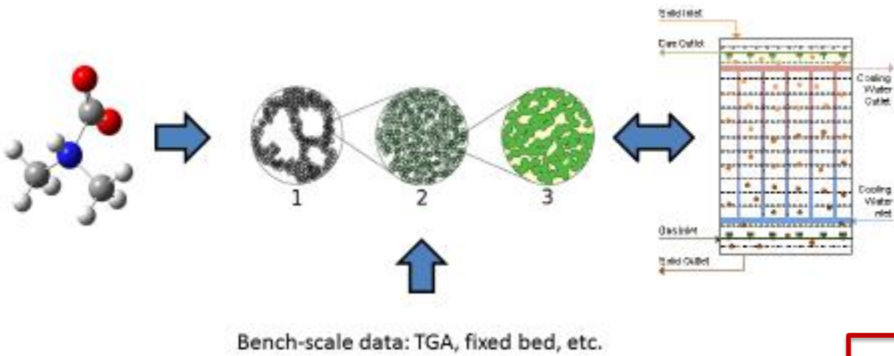
Screened tools

FOQUS Turbine and SimSinter

Process Models

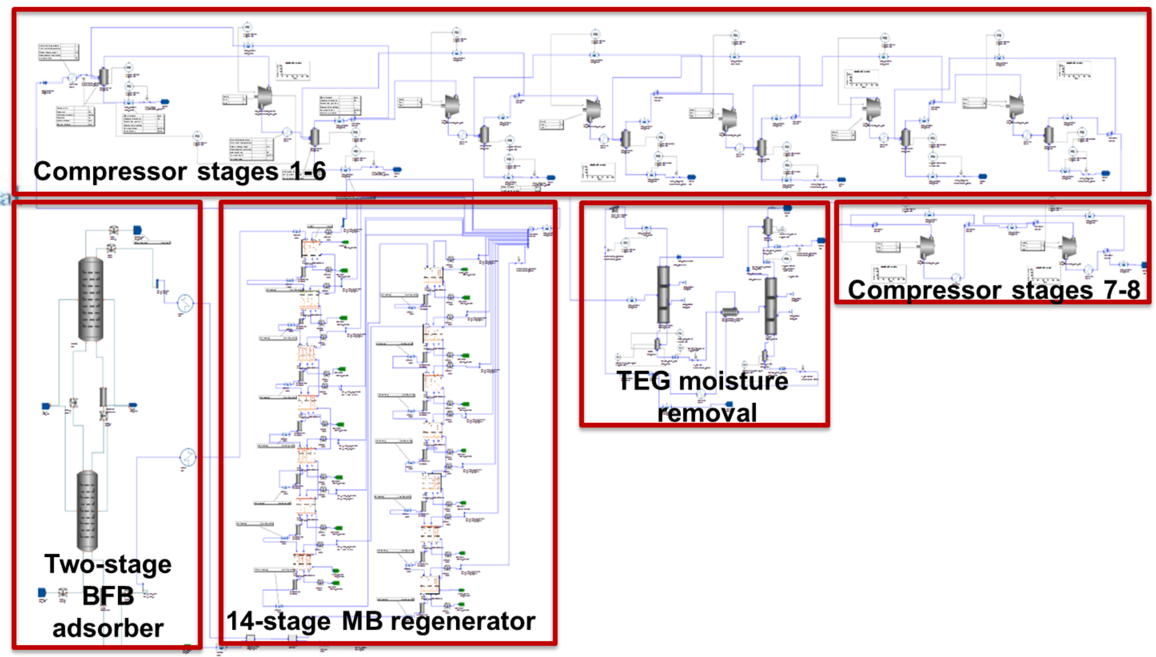
D. C. Miller, B. Ng, J. C. Eslick, C. Tong and Y. Chen, 2014, Advanced Computational Tools for Optimization and Uncertainty Quantification of Carbon Capture Processes. In *Proceedings of the 8th Foundations of Computer Aided Process Design Conference – FOCAPD 2014*. M. R. Eden, J. D. Siirola and G. P. Towler Elsevier.

WVU (Process Models)



Energy Systems and Materials Simulation

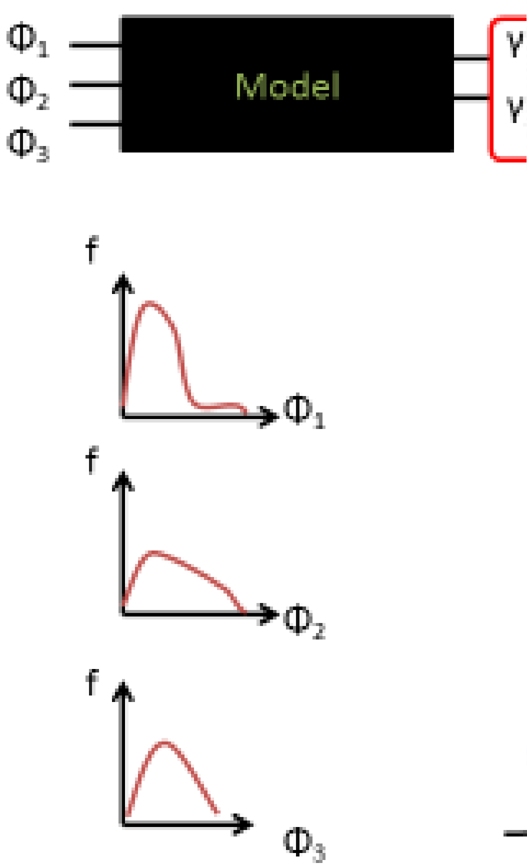
WestVirginia

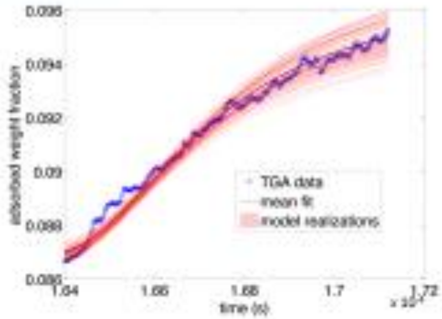


WVU (SorbentFit)

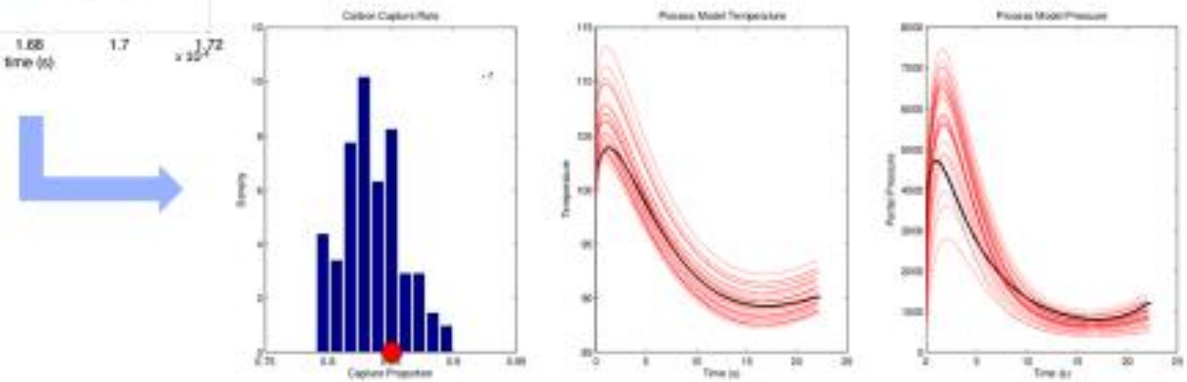
SorbentFit & SolventFit

Ba





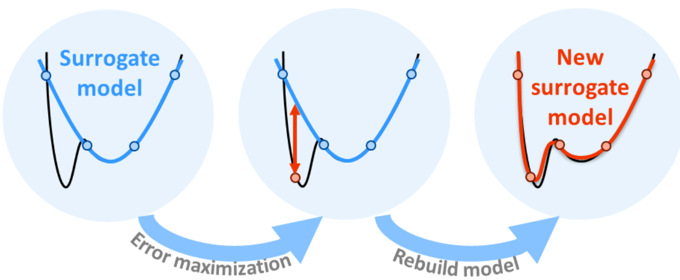
Top: Bayesian calibration of TGA sorbent data



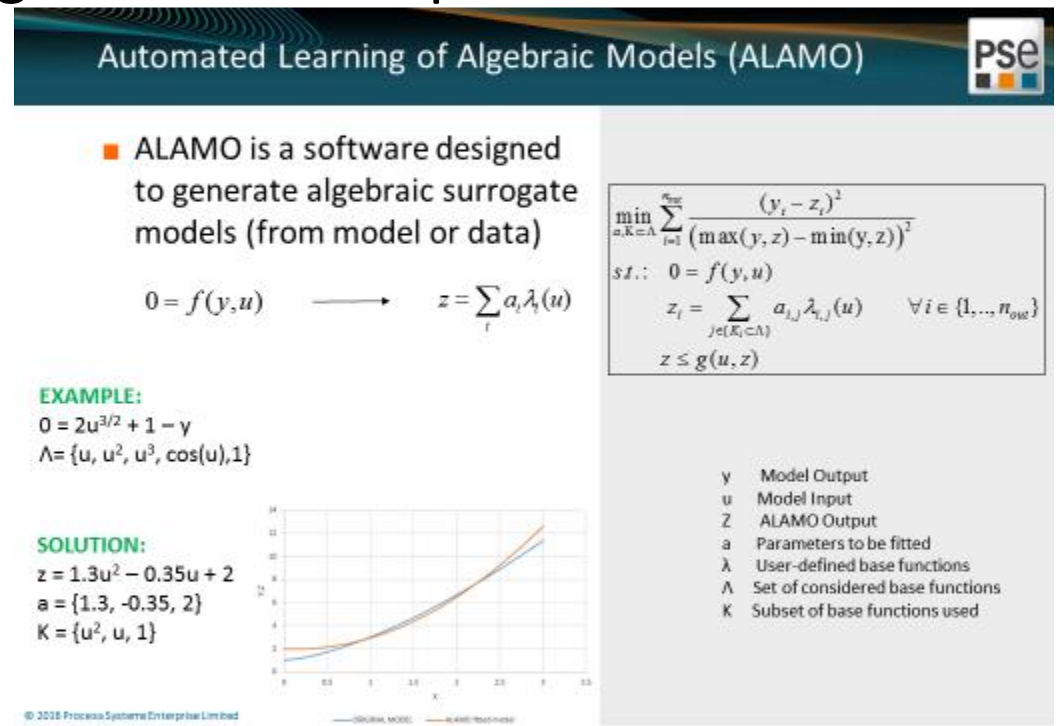
Bottom: Bubbling bed adsorber results. The "real" response of the system is the red dot / black curves.

parameter space.

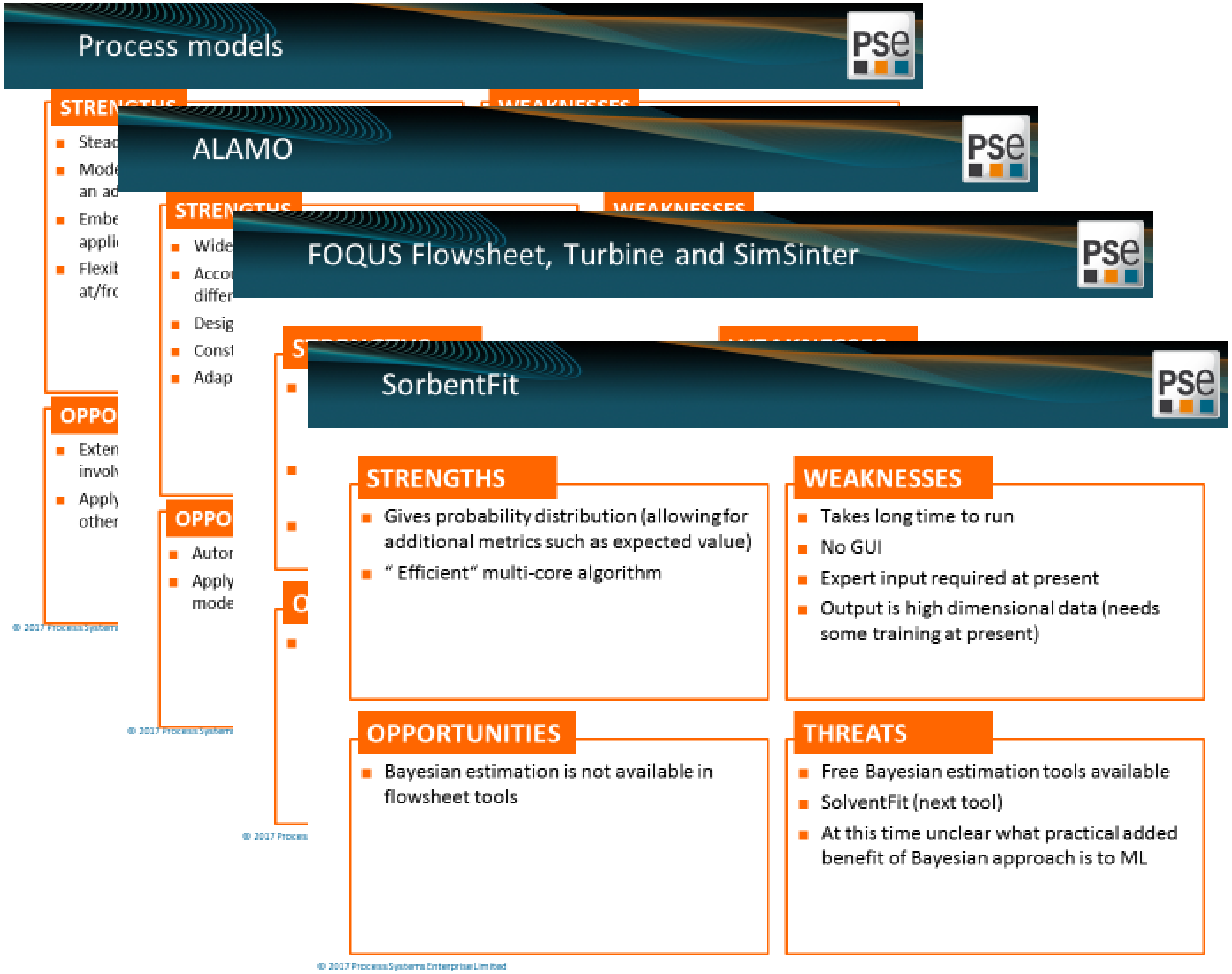
- Optimization-based machine learning methodology



- Capable of transforming data and complex models to algebraic models



SWOT ANALYSIS



Featured Opportunities

- Process Models: High fidelity gas-solid models could be extended to other process applications
- ALAMO: Could be used to speed up and automate UQ investigations
- FOQUS TURBINE: Parallelized simulations on cloud
- SorbentFit: Bayesian estimation provides unique capabilities

Assessment against commercialization criteria

		FOQUS Flowsheet and SimSinter	FOQUS Turbine	ALAMO	UQ module	Optimization Under Uncertainty	Dynamic Reduced Models	iREVEAL	Process Models	SorbentFit	Bayesian Calibration concepts
1	General applicability	2	7	6	3	3	4	1	4	1	7
2	User-friendliness	3	5	7	2	4	3	5	4	3	4
3	Impact on customer workflows	3	6	8	3	5	3	6	4	4	4
4	Alignment with platform	3	6	7	5	6	6	6	6	5	7
5	Perceived estimated market	3	8	7	4	4	4	4	4	2	8
6	Technical Advance Level	6	7	6	7	8	4	6	4	8	8
7	Technical Readiness Level	4	5	7	4	5	5	6	7	4	5
8	Commercial Readiness Level	3	7	7	3	4	4	5	5	3	5
9	Required development	3	5	7	3	5	4	5	5	4	5
10	Support / maintenance required	2	5	7	4	5	6	5	6	4	6

Feedback from potential customers

"ability to use with commercial simulators is a plus"

"Complex work flow"

"Improve user friendliness"

"Limited scope"

"**Need to demonstration value**"

"Why change?"

"Concerned about long-term support"

"Simulation time"

"cutting-edge technology"

"certain tools can be used outside CCS"

The Carbon Capture Simulation Initiative (CCSI) commercialization project

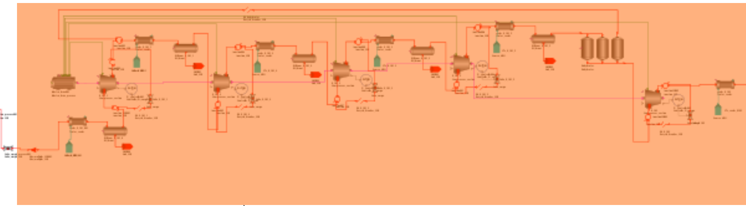
Case studies: Improving commercial potential

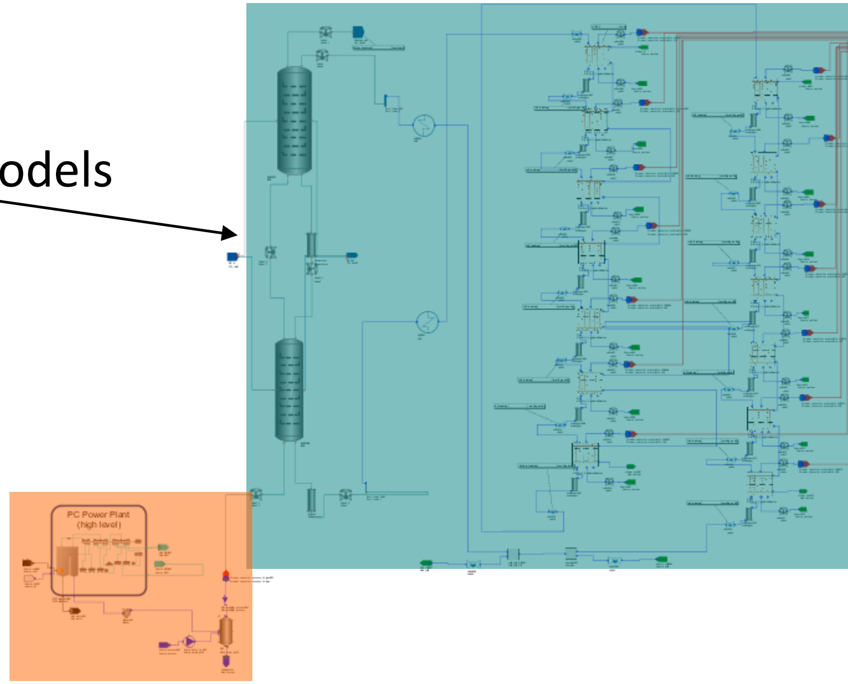
Extending model scope

CCSI BFB and MB models

gCCS Power plant

gCCS CO_2 Compression





Fixed bed model developed

H_2 purification model validation

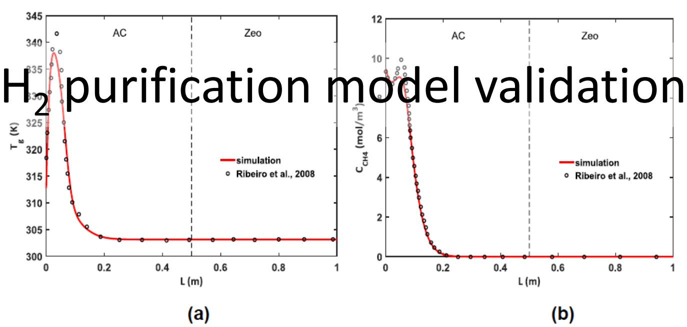


Figure 8. **(a)** Gas temperature profile and **(b)** methane gas concentration profile at the end of the feed step (simulation time t = 40 s), as a function of bed length. Simulation results compared to results published by Ribeiro et al. (2008)

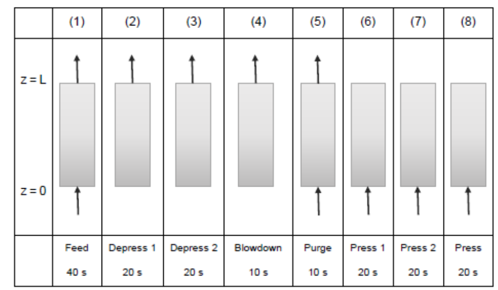


Figure 9 Schematic diagram of the cycle sequence used for the PSA simulation.

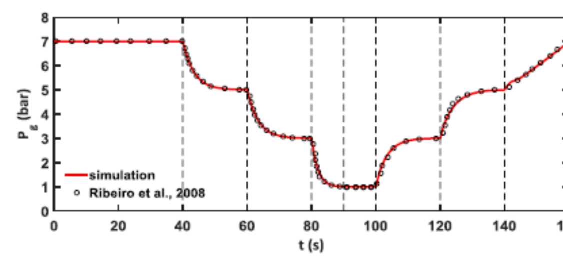


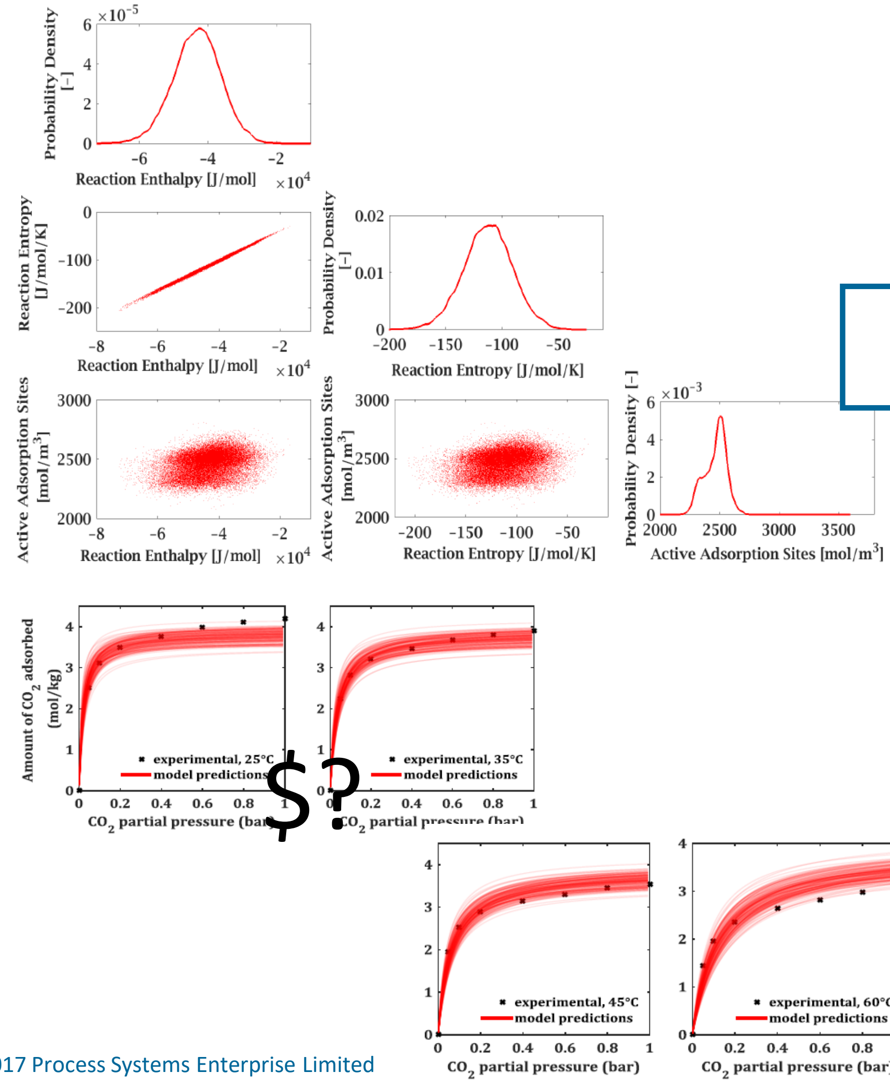
Figure 10 Pressure at the reactor outlet – comparison between simulation results and results published by Ribeiro et al. (2008)

Demonstrations – value of improved model calibration

Results – Langmuir Model Calibration

West Virginia University

Parameter uncertainty only, $\boldsymbol{\theta} = [\Delta H, \Delta S, n_v]$



$?

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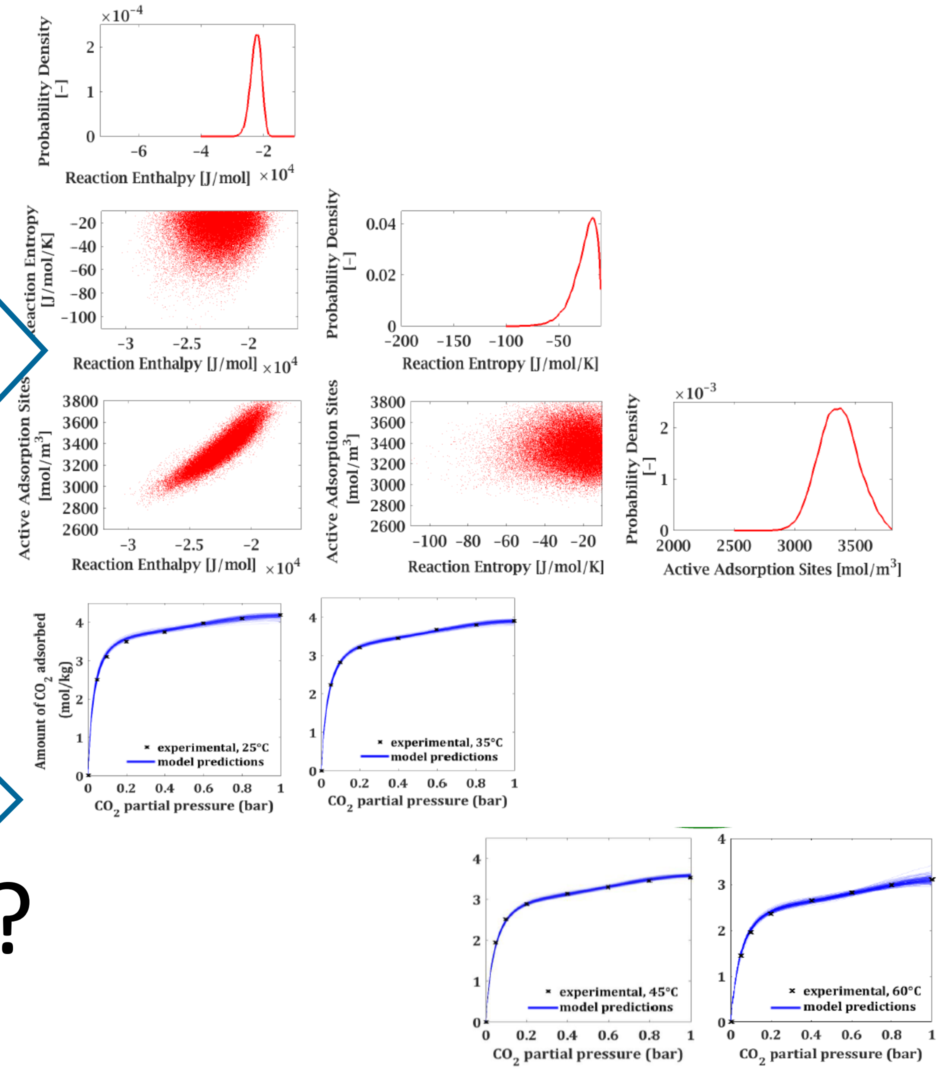
Results – Langmuir Model Calibration

West Virginia University

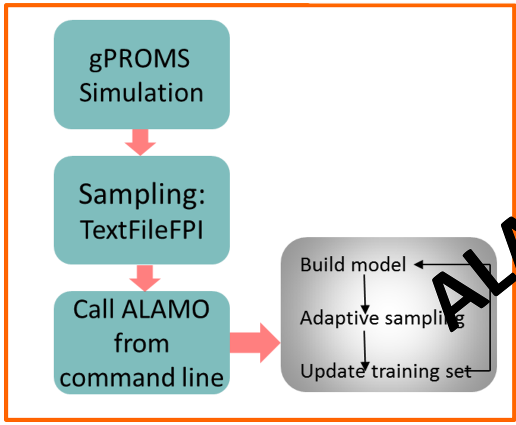
Parameter uncertainty and model discrepancy, $\boldsymbol{\theta} = [\Delta H, \Delta S, n_v]$ and $\boldsymbol{\delta}$



Proposal for improving workflows and usability

ALAMO

Now

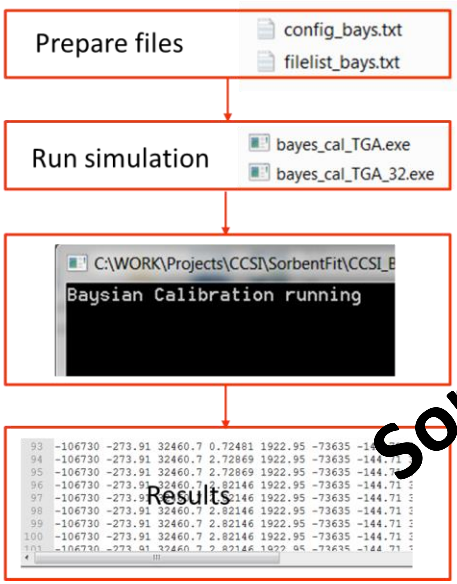


Possible commercialization

- Run ALAMO within gPROMS

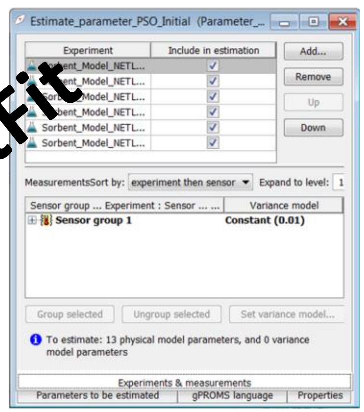
SorbentFit

Now



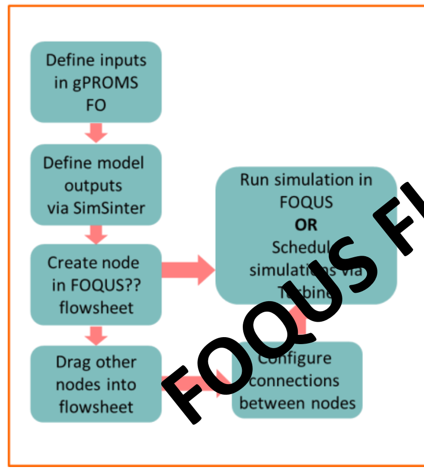
Possible commercialization

- Integrate with gPROMS parameter estimation entity
- Create GUI

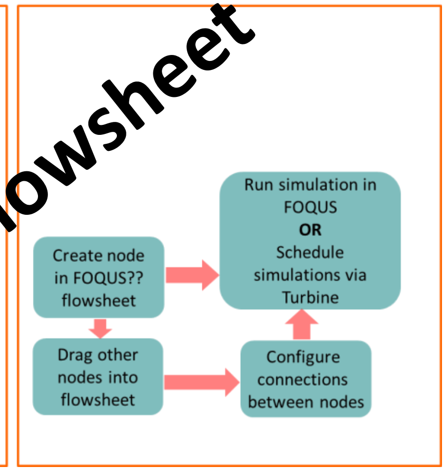


FOQUS Flowsheet

Now



Possible commercialization



Summary

- PSE has assessed the CCSI toolset for commercialization within its advanced modelling platform, gPROMS
- The CCSI toolset represents cutting-edge research in the development of CCS
- PSE has identified and proposed development areas for the commercialization of the tools especially with regards usability and demonstration of additional value
- PSE will continue to support the $CCSI^2$ project

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- Lawrence Berkeley National Laboratory: Deb Agarwal and Josh Boverhoff
- The entire project team

Thank you