ADVANCED PROCESS MODELING FORUM **2014**

gCCS

An integrated modeling environment for whole-chain CCS systems

Alfredo Ramos – VP Power & CCS Business Unit

What is CCS?

Carbon Capture & Storage – technology and stakeholders

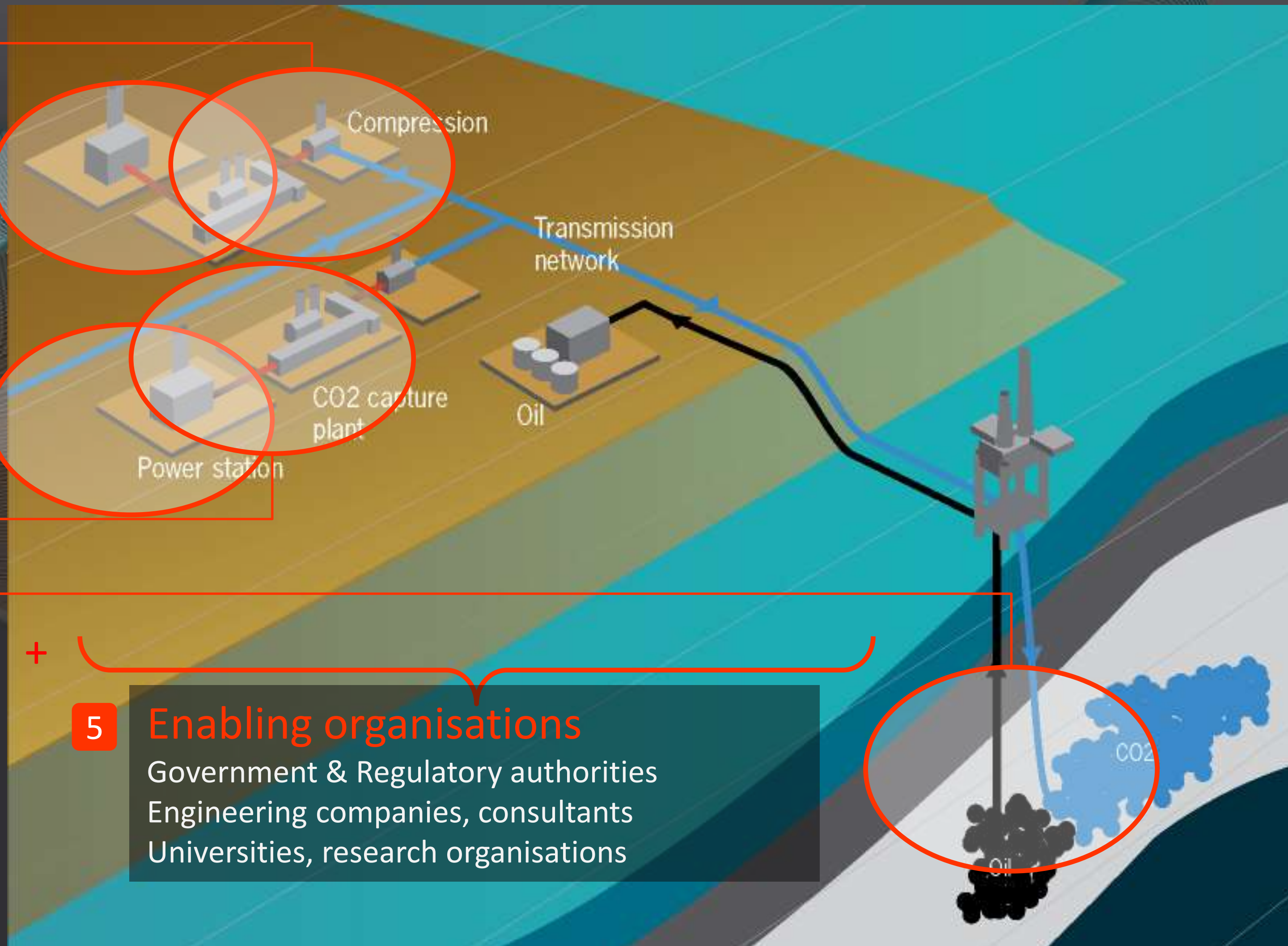
3 Compression & transmission

2 Industrial gas companies

1 Power generators

2 Process providers

4 Storage providers



5 **Enabling organisations**

Government & Regulatory authorities
Engineering companies, consultants
Universities, research organisations

Climate change

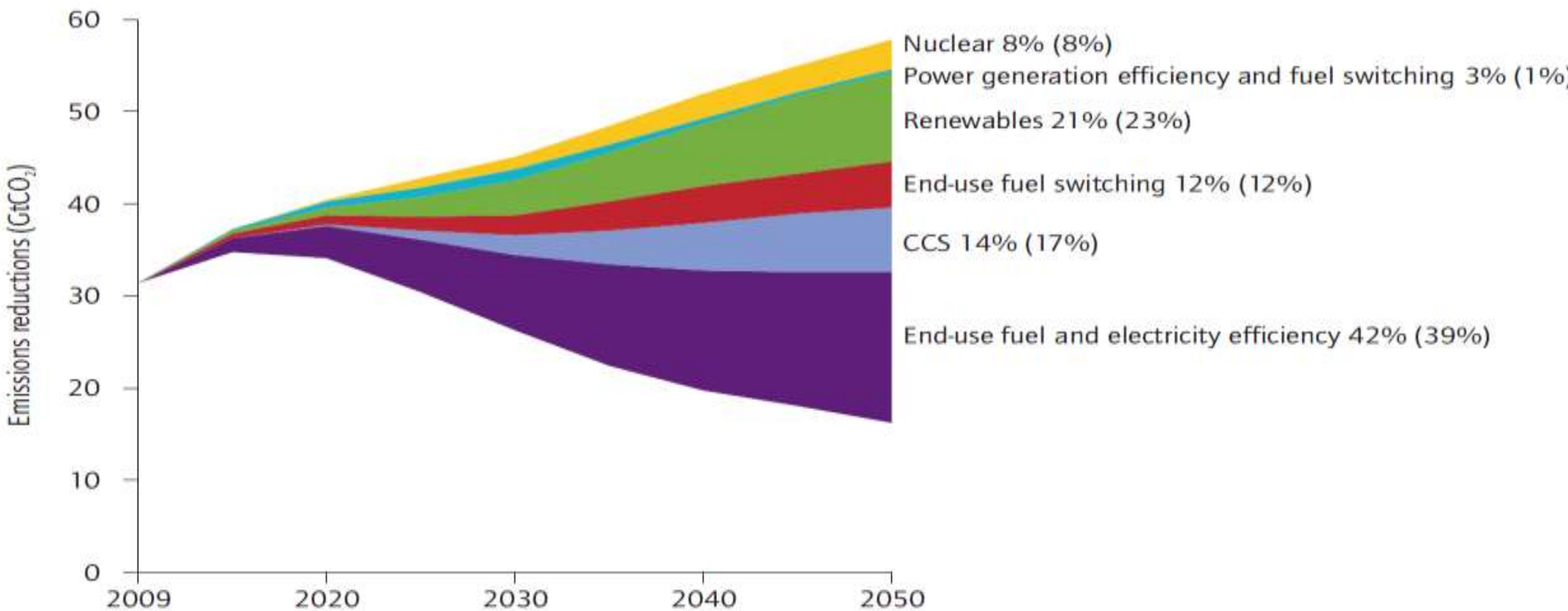
- The world's leading scientists have warned that unless the rise in average **global temperature is kept below 2°C**, devastating and irreversible climate change will occur
  - likely uncertainty range of 1.6-2.6 °C

Allen, M. R. et al (2009) *Warming caused by cumulative carbon emissions towards the trillionth tonne*, Nature, 458:1163-1166
Meinshausen, M. et al (2009) *Greenhouse gas emission targets for limiting global warming to 2 °C*, Nature, 458:1158-1162

Optimal energy generation portfolio (I)

- From a global perspective…

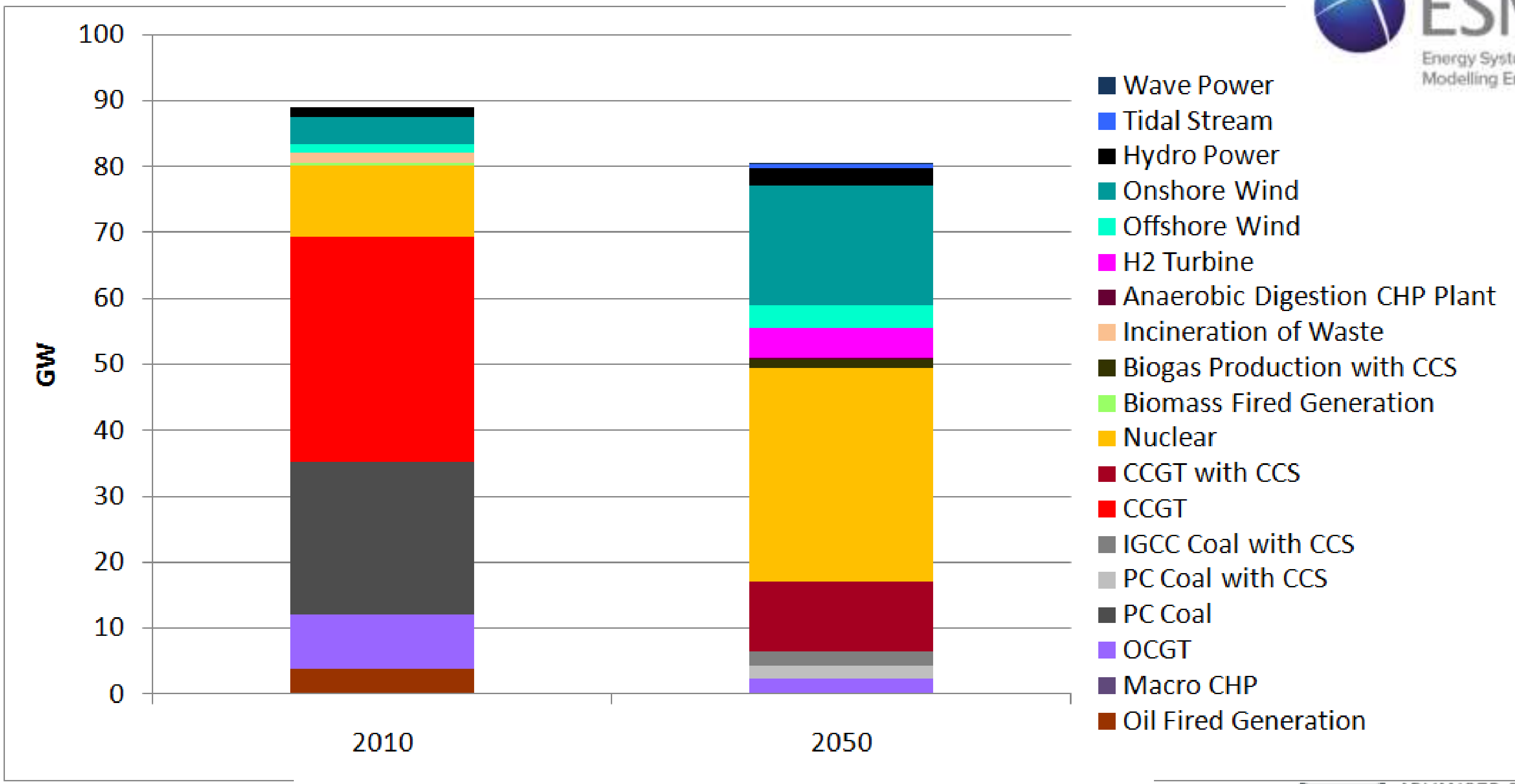
Source: International Energy Agency (IEA)



- IEA Conclusions:
  - Attempting to address emissions without CCS raises costs by 40% (a total extra cost of $2 trillion over 40 years)
  - Milestones: 30 projects by 2020 & 120Gt of CO2 stored by 2050

Optimal energy generation portfolio (II)

- ...to an UK view
  - 2050 power generating capacity: Energy mix optimised for achieving energy security and GHG emission targets



Source: Energy Technologies Institute (ETI)

Summary

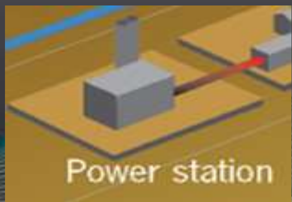
- Tackling climate change without CCS will be more expensive
- Low carbon fossil fuel power stations with CCS are complimentary to intermittent renewables and inflexible nuclear energy
- Furthermore, CCS is applicable to industrial sources of carbon dioxide (CO2), not just fossil-fuelled power plant

CCS systems

Existing technology in a new configuration

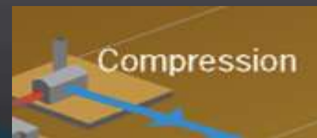
Project developers & Financial institutions
Risk analysis
Liabilities
Contracts

Government
Policy
Strategic
Infrastructure development
H&S



Grid demand
Flexibility
Efficiency
Fuel mix
Trip scenarios

Sizing
Flexibility
Buffer storage
Amine loading
Capital cost optimisation
Energy sacrifice
Heat integration
Solvent issues



Optimal operating point
Efficiency
New design
Impurities
Control
Safety

Composition effects
Phase behavior
Capacity
Buffering / packing
Routing
Safety
Depressurisation
Control
Leak detection

Compression
Supply variability
Composition
Thermodynamics
Temperatures / hydrates
Well performance
Long-term storage dynamics
Back-pressures

Cannot be assessed in isolation in an integrated CCS system

System-wide modelling

Key enabling technology for CCS

- Explore **complex decision space** rapidly based on high-fidelity, technically realistic models
  - resolve own technical and economic issues
  - take into account upstream & downstream behaviour
  - Manage **interactions** and **trade-offs**
- **Evaluate technology** – existing and next-generation
  - judge relative merits of emerging technologies
  - support consistent, future-proof choices
- **Integrating platform** for
  - working with other stakeholders in chain
  - collaborative R&D, working with academia

The CCS System modelling Tool-kit Project

Sept 2011 – Jun 2014

energy technologies institute

- **Energy Technologies Institute (ETI)**

corporate

public institutions

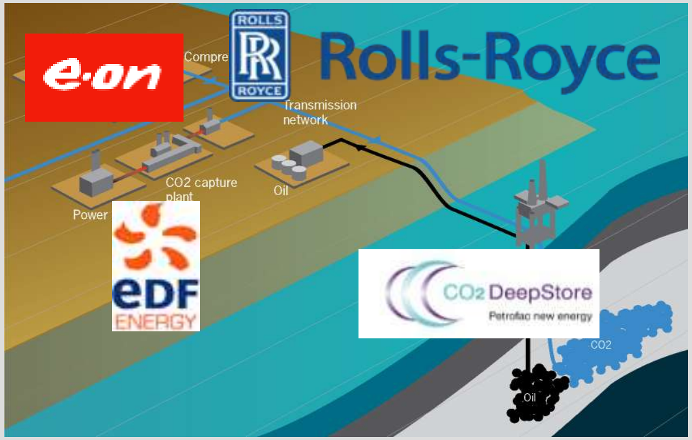
Department of Energy & Climate Change

Technology Strategy Board

– ~$5m project commissioned & co-funded by the ETI

– Objective: **"end-to-end" CCS modelling tool**

gCCS



PSE

gPROMS modelling platform & expertise

E4tech

Project Management

Project objectives

Develop a Modelling Toolkit

capable of modelling the operation

of full-chain CCS systems or subsets of such systems

End-to-end
Model-Based Decision Support

gCCS v1.0

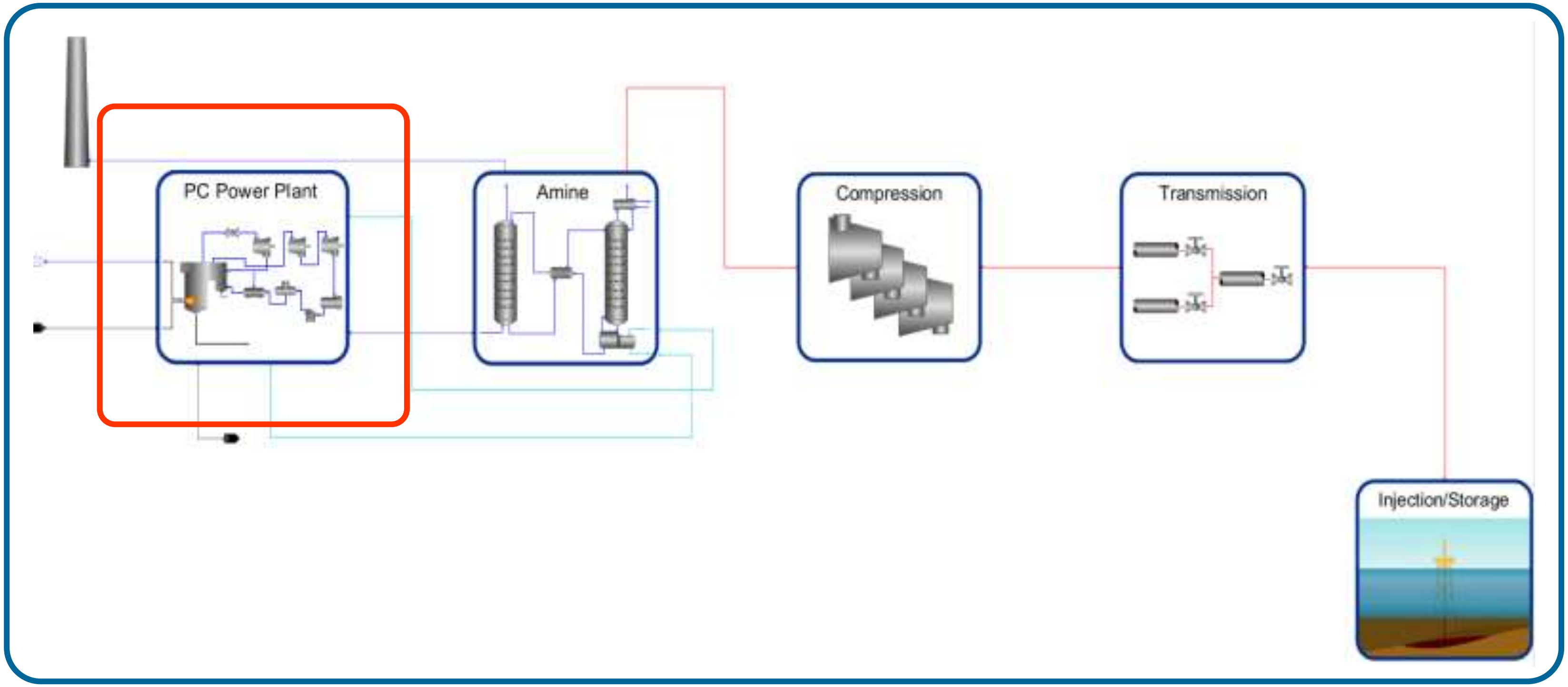
gCCS initial scope (2014/Q3)

- **Process models**
  - Power generation
    - Conventional: pulverised-coal, CCGT
    - Non-conventional: oxy-fuelled, IGCC
  - Solvent-based CO_2 capture
  - CO_2 compression & liquefaction
  - CO_2 transportation
  - CO_2 injection in sub-sea storage

- **Materials models**
  - cubic EoS (PR 78)
    - flue gas in power plant
  - Corresponding States Model
    - water/steam streams
  - SAFT-VR SW/ SAFT-γ Mie
    - amine-containing streams in CO_2 capture
  - SAFT-γ Mie
    - near-pure post-capture CO_2 streams

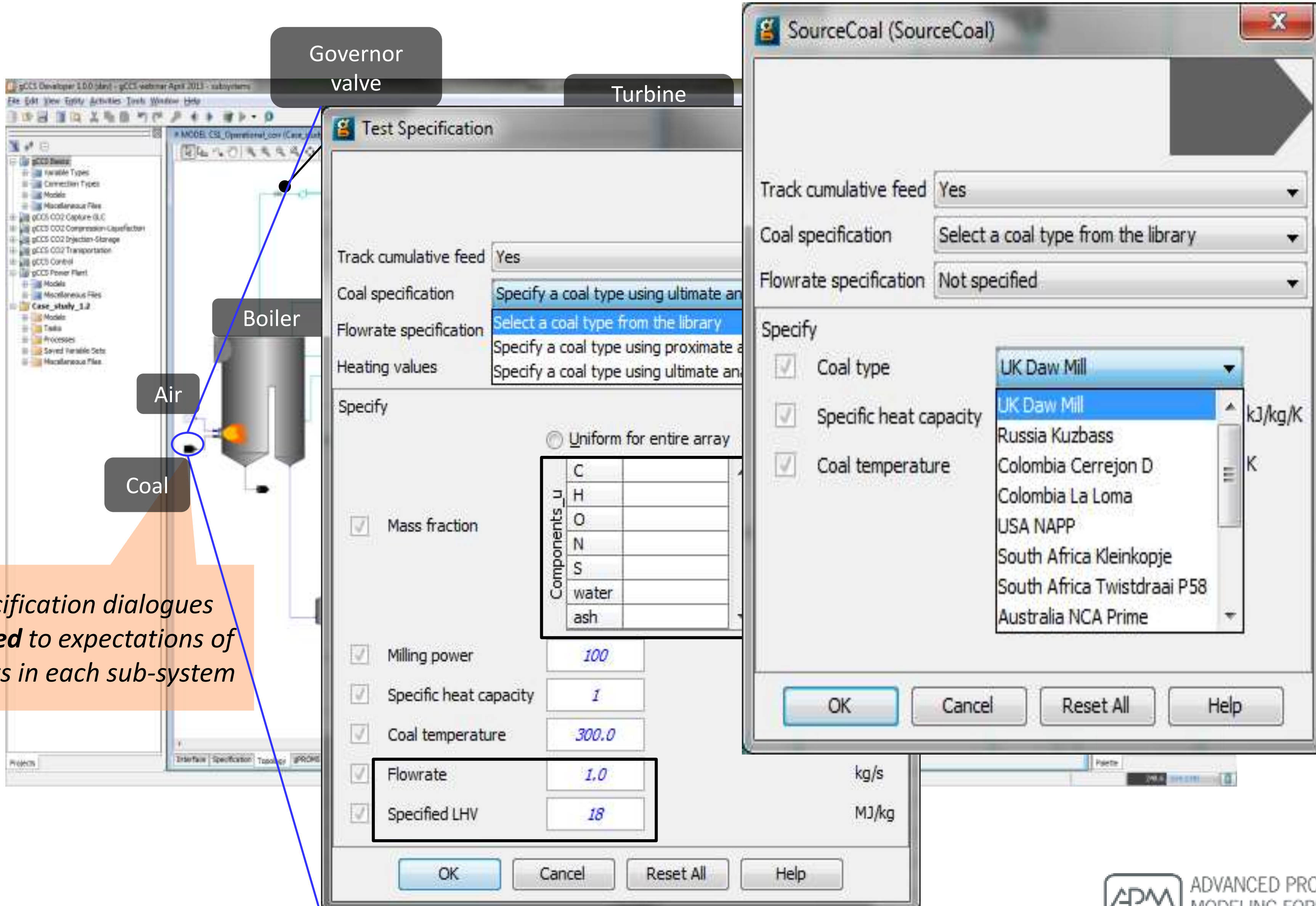
Open architecture allows incorporation of 3rd party models (e.g. E.ON's PROATES)

Power generation



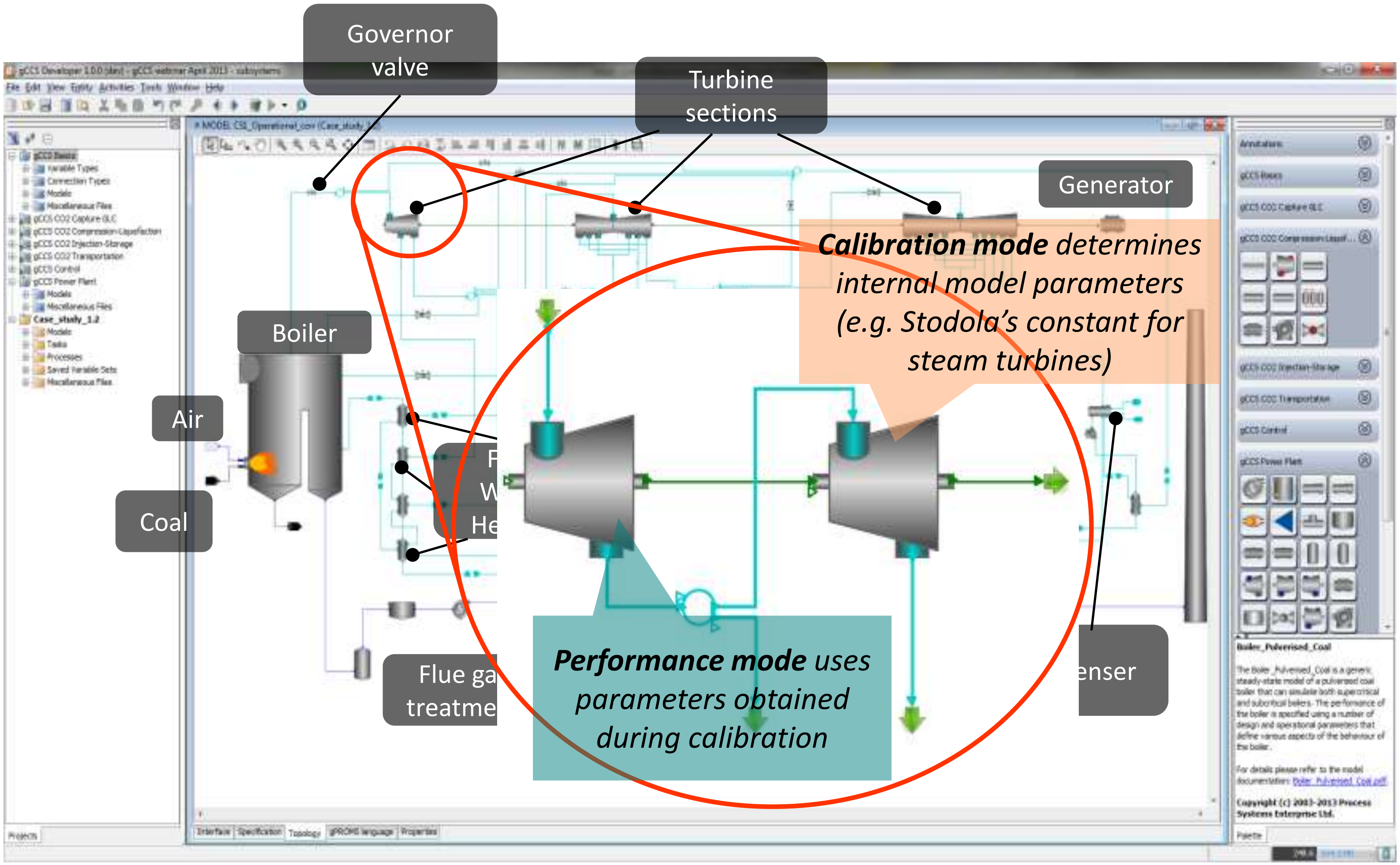
gCCS Power Plant Library

Features

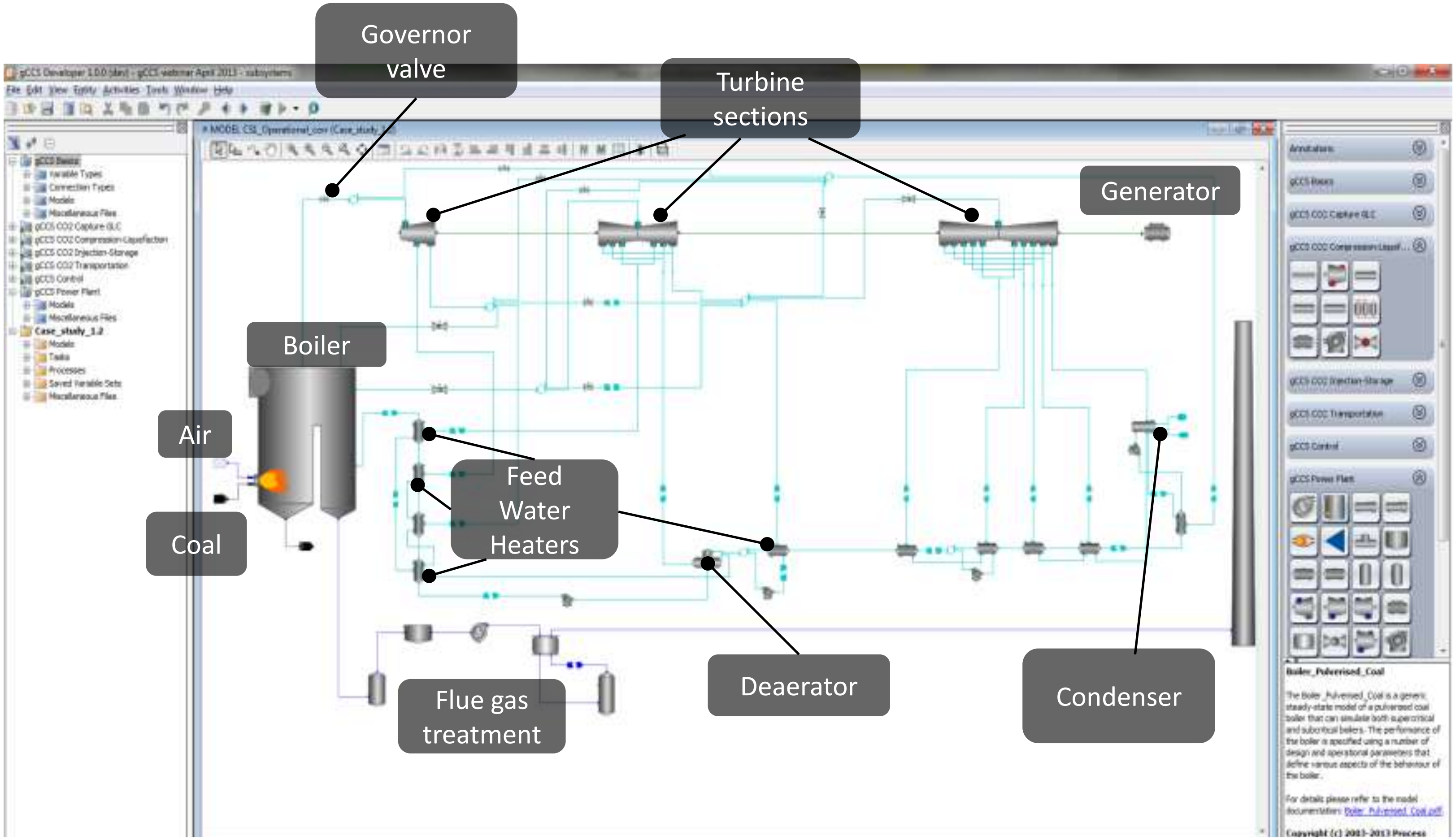


Specification dialogues ***tailored*** *to expectations of experts in each sub-system*

Features


Governor valve
Turbine sections
Generator
Boiler
Air
Coal
Flue ga
treatme
enser
Calibration mode determines internal model parameters (e.g. Stodola's constant for steam turbines)
Performance mode uses parameters obtained during calibration

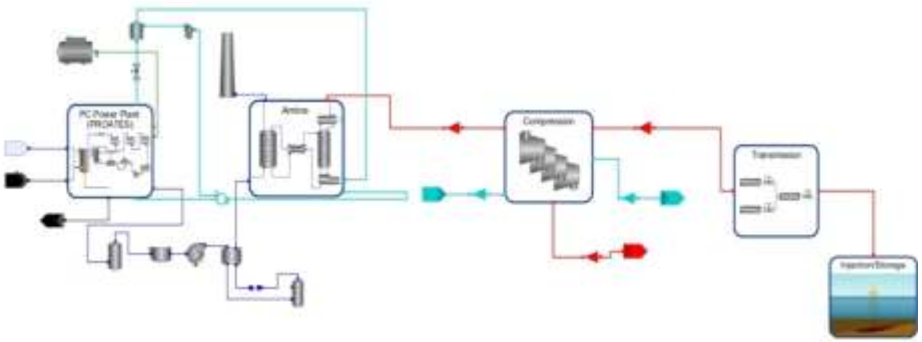
Features



Complex flowsheet with > 10 recycles & a closed loop:
→ Component-specific initialisation procedures ensure convergence **with minimum provision of initial guesses**

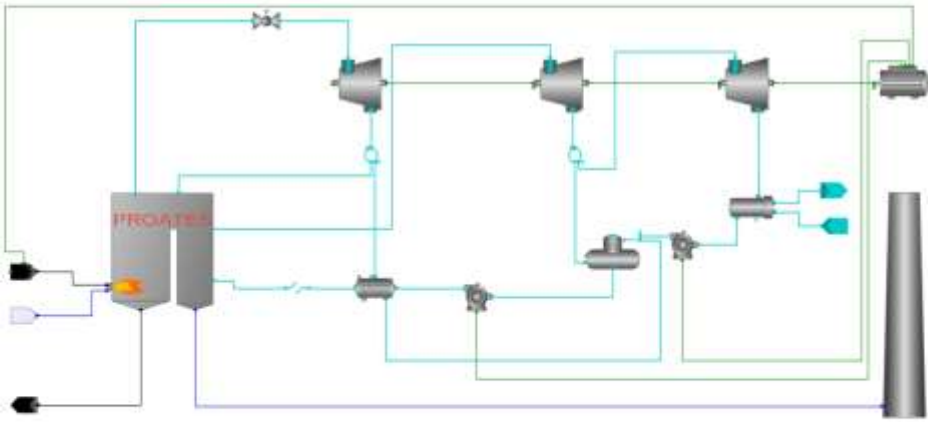
Interfaces to 3rd party modelling tools

1) PROATES power plant integrated in CCS chain



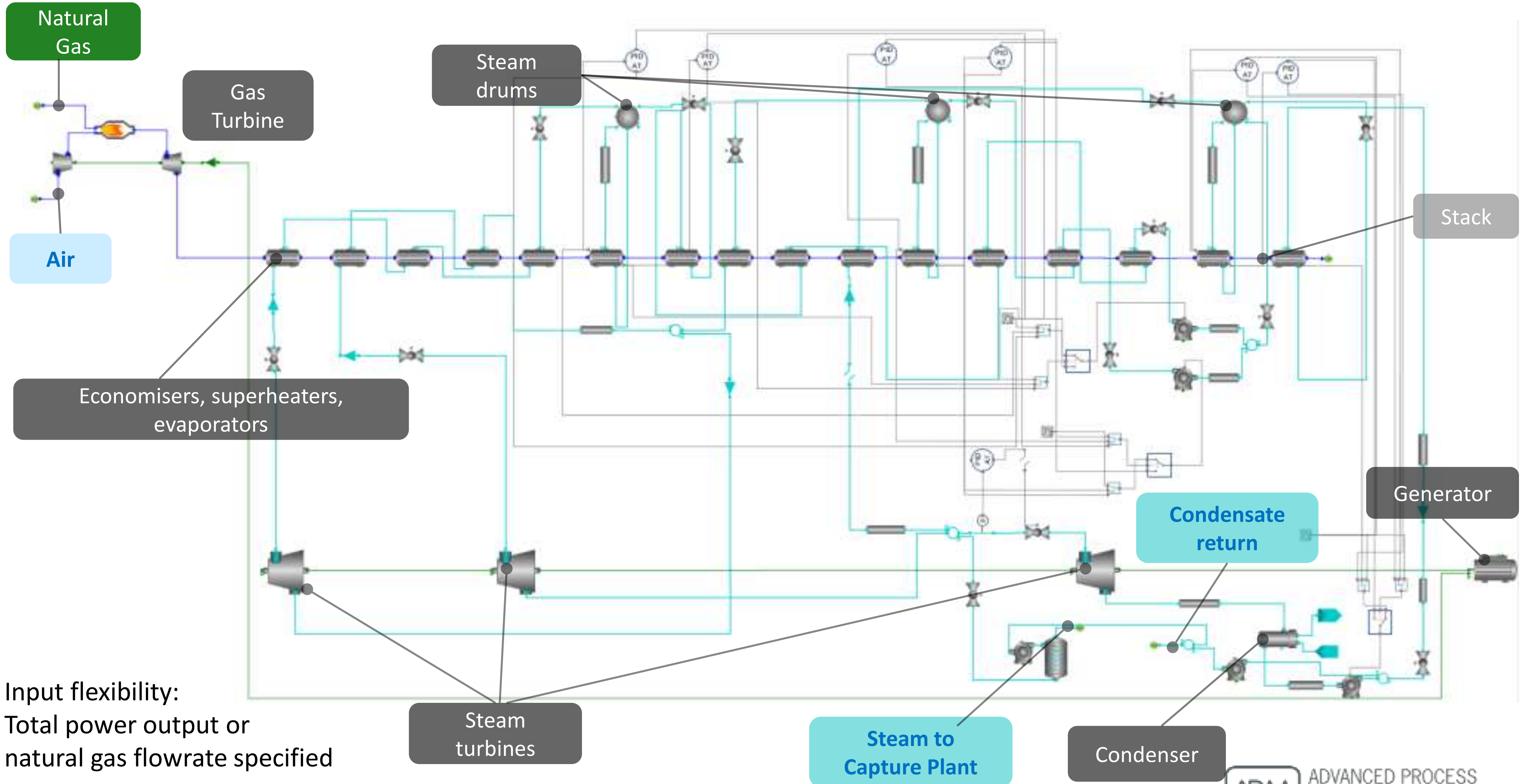
	Unit	gCCS Case Study 1	PROATES & gCCS Case Study 2	Deviation (%)
Gross power output without capture	MW_e	819.00	819.00	0.00
Gross power output with capture	MW_e	696.65	703.60	-0.99
Gross efficiency without capture	% LHV	49.41	49.40	0.02
Gross efficiency with capture	% LHV	41.97	42.41	-1.04
Net Power output with capture	MW_e	602.56	615.16	-2.05
Net efficiency with capture	% LHV	36.35	37.09	-2.00

2) PROATES boiler integrated in gCCS power plant



	PROATES	gCCS	Deviation [%]
Load [MW]	450.03	450.27	0.05
CO_2 mass fraction in flue gas [-]	0.19	0.19	0.42
Flue gas mass flowrate [kg/s]	603.03	599.63	-0.56
Combustion air mass flowrate [kg/s]	554.77	551.32	-0.62
Feedwater mass flowrate [kg/s]	393.65	393.94	0.07
Flue gas temperature [°C]	395.09	123.33	1.39

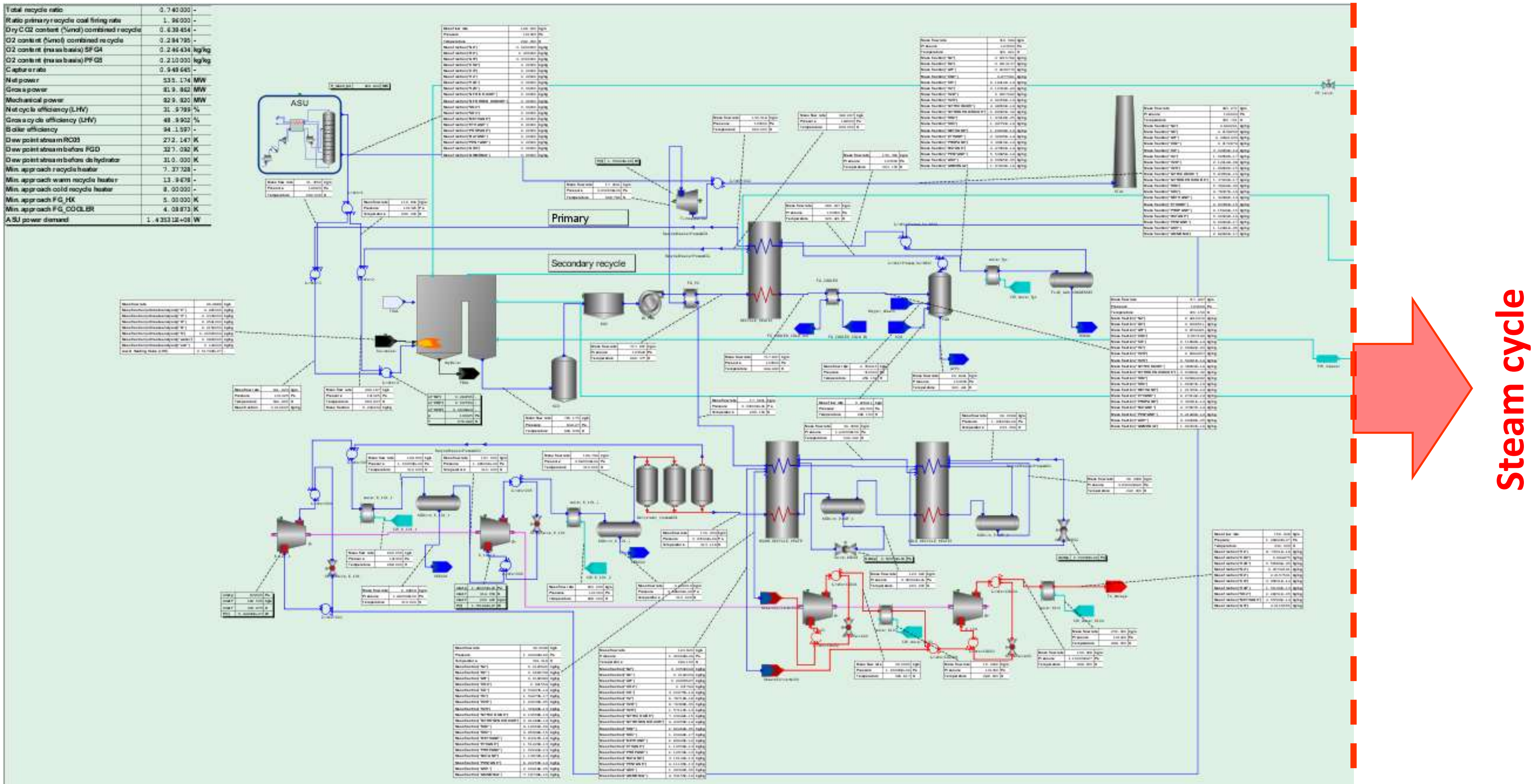
CCGT power plant



Input flexibility:
Total power output or
natural gas flowrate specified

Oxyfuel power plant

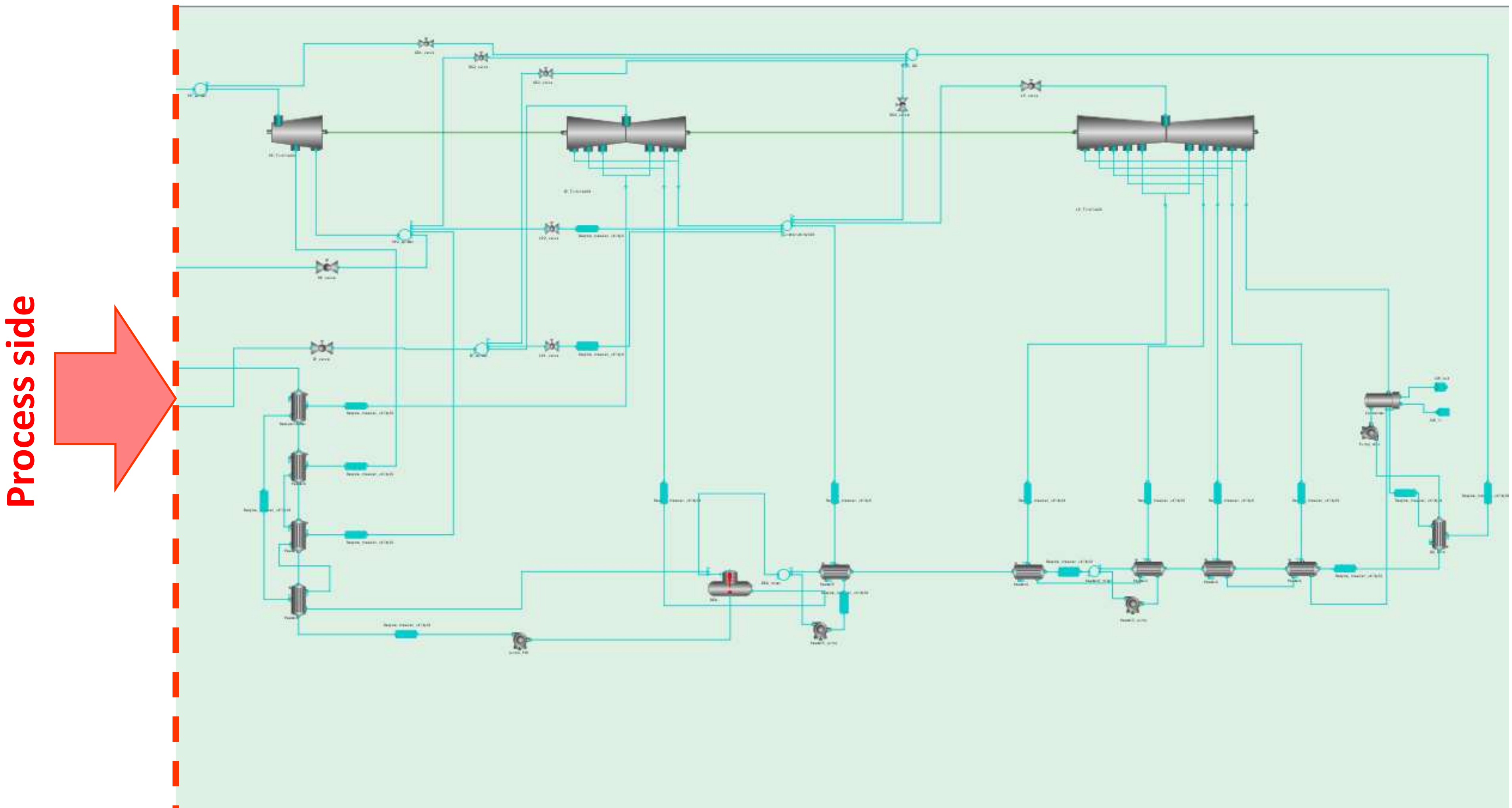
- Process side



Total recycle ratio	0.740000	-
Ratio primary recycle coal firing rate	1.96000	-
Dry CO2 content (%mol) combined recycle	0.638454	-
O2 content (%mol) combined recycle	0.284795	-
O2 content (mass basis) SFG4	0.246434	kg/kg
O2 content (mass basis) PFG5	0.210000	kg/kg
Capture ratio	0.948645	-
Net power	535.174	MW
Gross power	819.862	MW
Mechanical power	829.820	MW
Net cycle efficiency (LHV)	31.9789	%
Gross cycle efficiency (LHV)	48.9902	%
Boiler efficiency	94.1597	-
Dew point stream RC05	272.147	K
Dew point stream before FGD	327.092	K
Dew point stream before dehydrator	310.000	K
Min. approach recycle heater	7.37728	-
Min. approach warm recycle heater	13.9678	-
Min. approach cold recycle heater	8.00000	-
Min. approach FG_HX	5.00000	K
Min. approach FG_COOLER	4.08873	K
ASU power demand	1.43531E+08	W

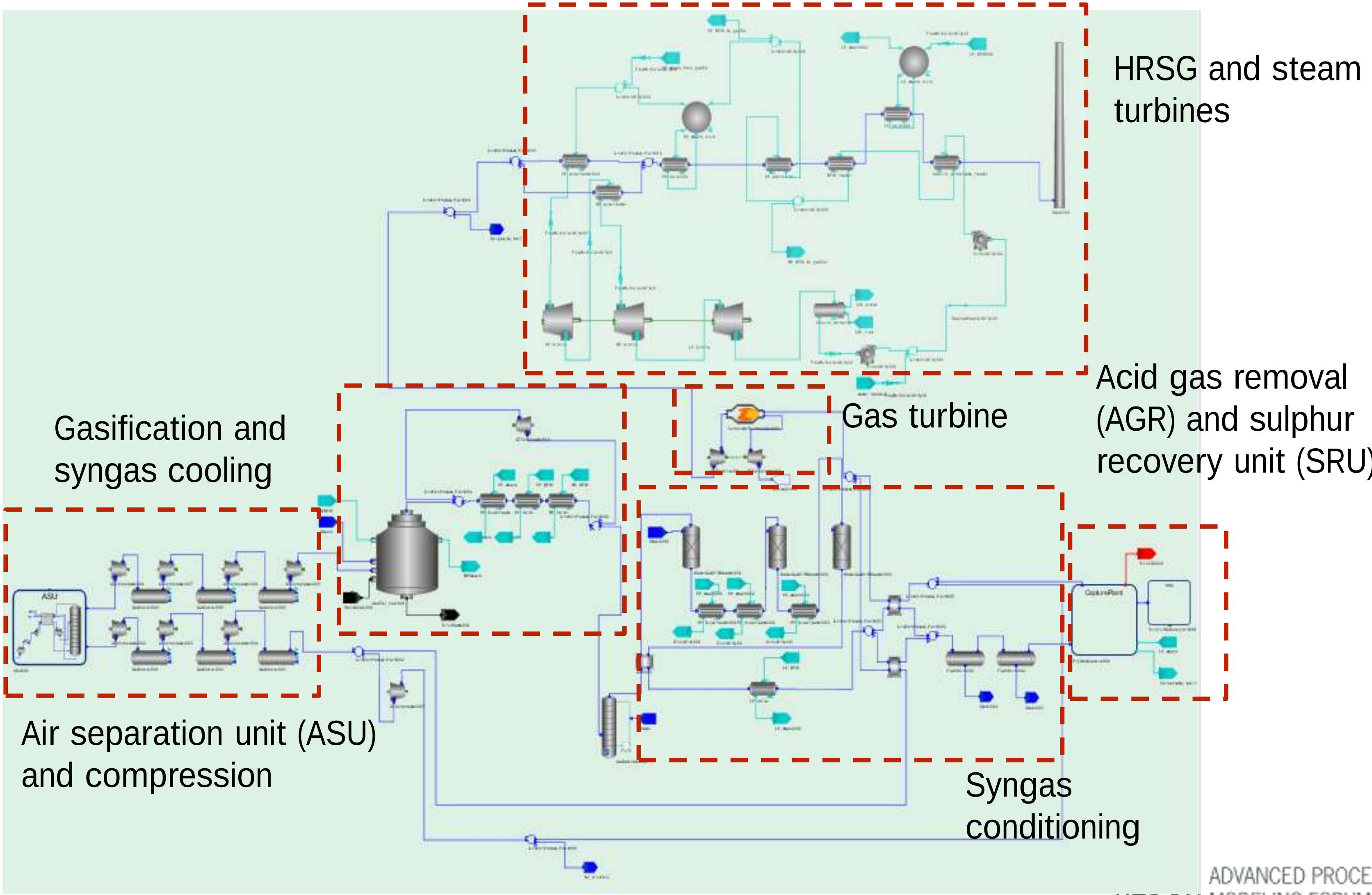
Oxyfuel power plant

- Steam Cycle

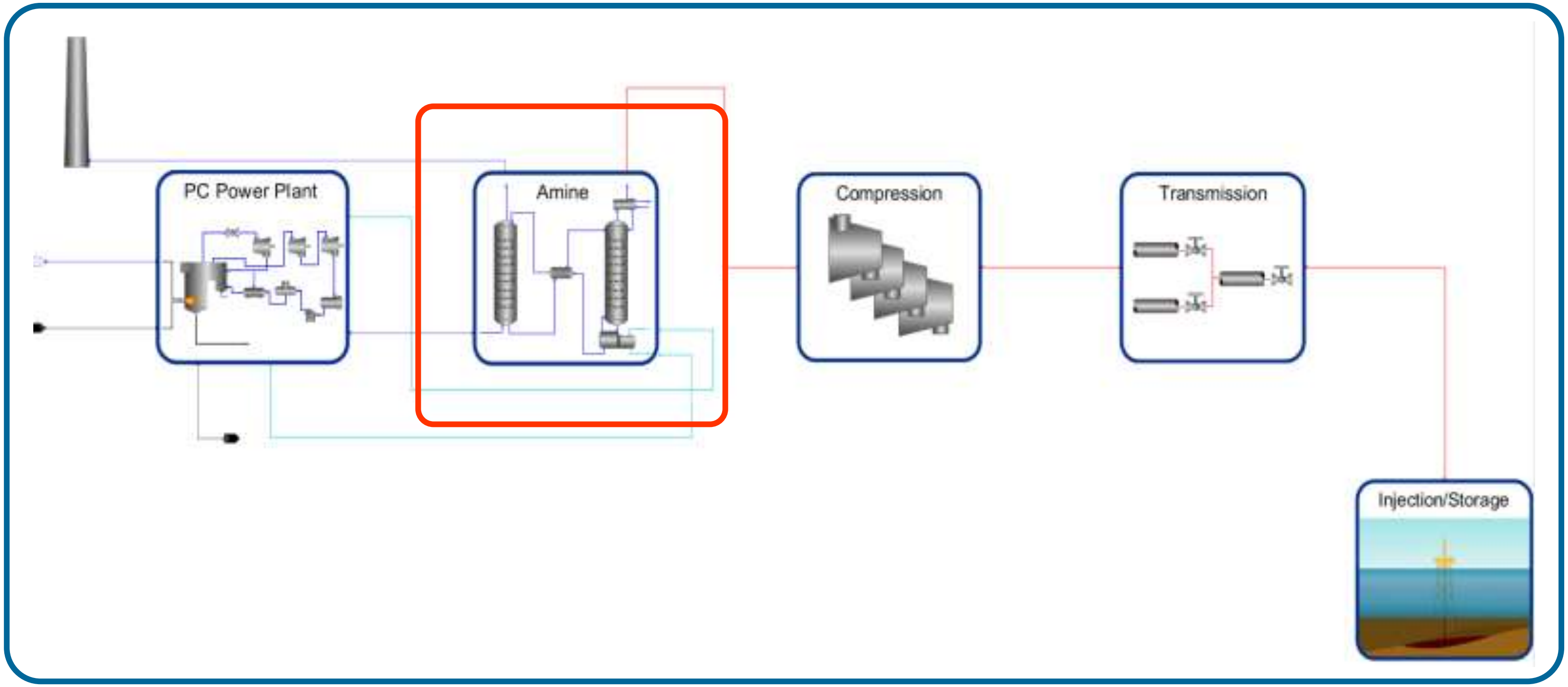


Non-Conventional Generation

- Integrated Gasification Combined Cycle power plant (IGCC)



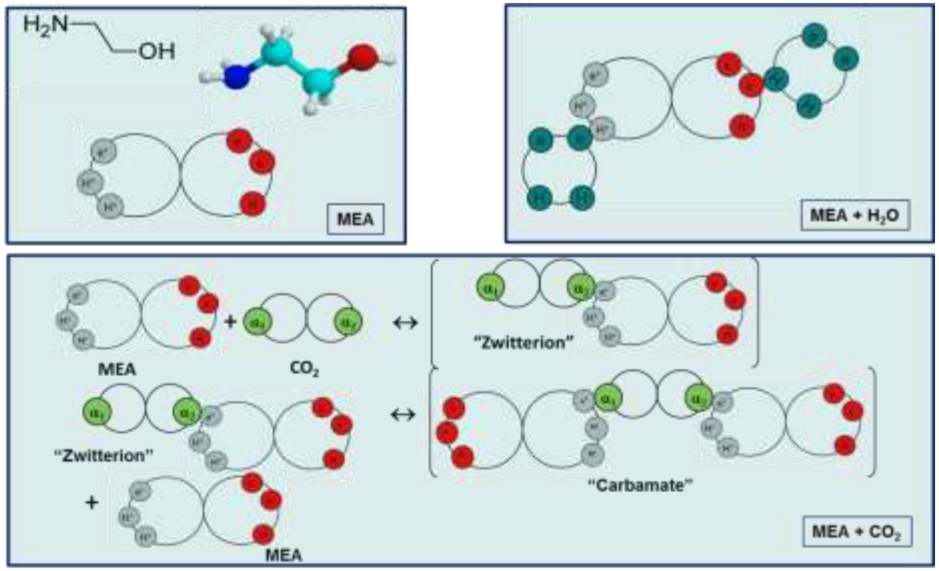
CO_2 Capture
Chemical and physical absorption



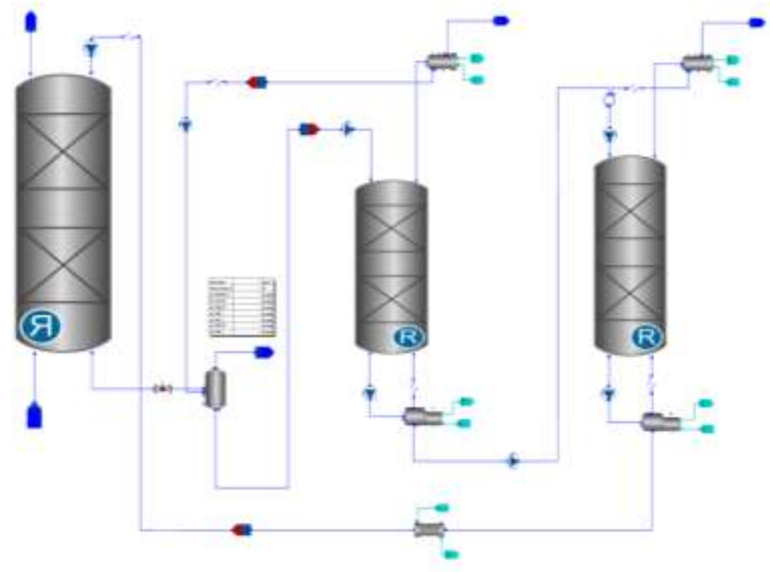
gCCS CO_2 Capture library

gSAFT material models

- chemical absorption
- physical absorption



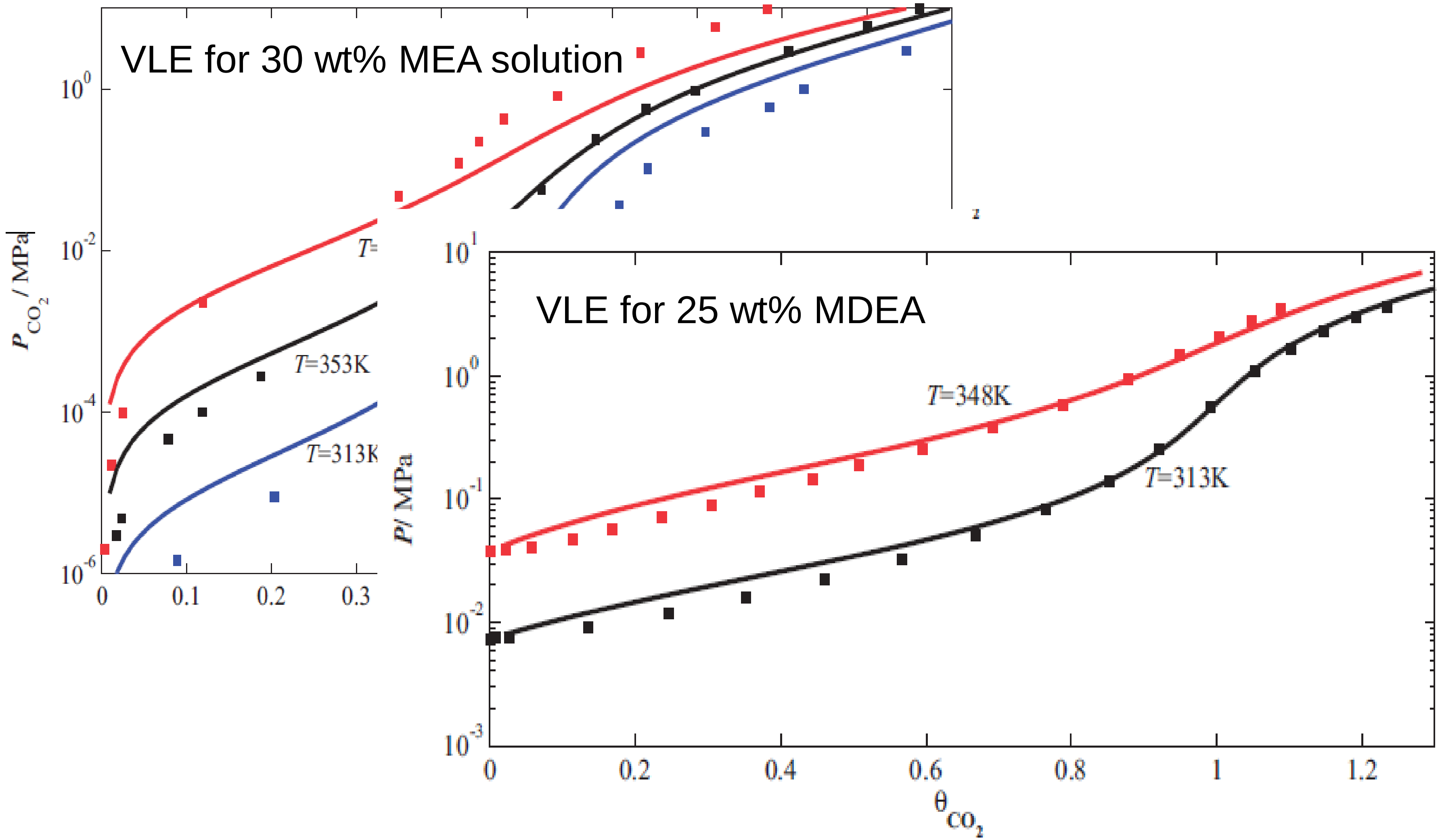
gCCS process models



Material models for chemical absorption

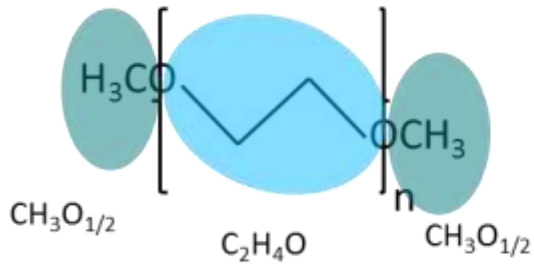
- Based on SAFT-VR SW equation of state
  - Well proven
  - Suitable for reacting systems
    - Chemical reactions are treated implicitly
    - Reaction products treated as aggregates of the reactant molecules
- gSAFT thermodynamic models available for
  - MEA, aMDEA/MDEA, NH_3
    - based on sound thermodynamic data

Material models for chemical absorption



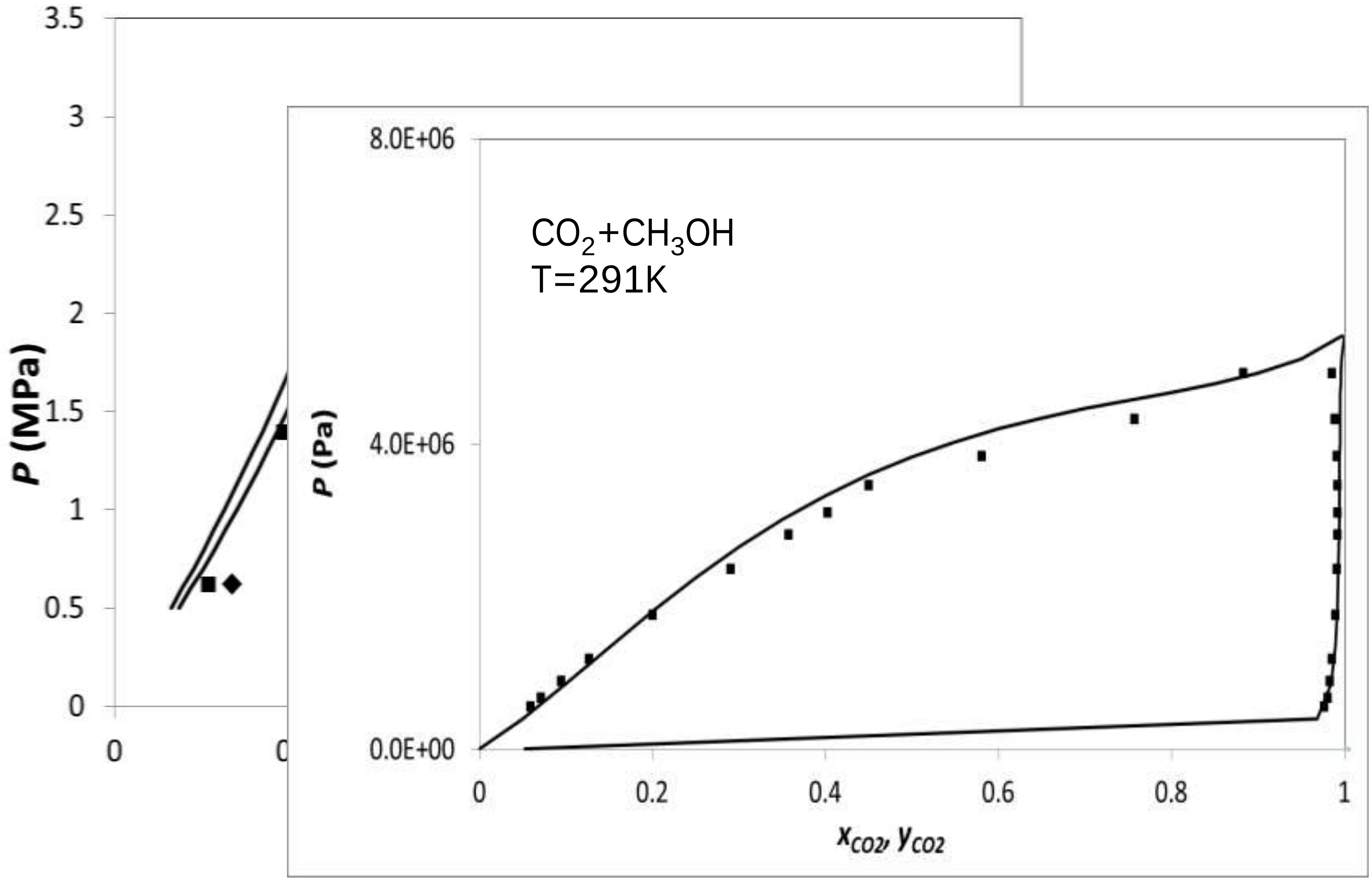
Material models for physical absorption

- Based on SAFT-γ Mie equation of state
  - Group contribution
- gSAFT thermodynamic models available for
  - Rectisol
    - Methanol as solvent
    - Model based on sound experimental data
  - Selexol
    - A mixture of PEGDMEs as solvent
    - Used group contribution method to develop thermodynamic model from experimental data

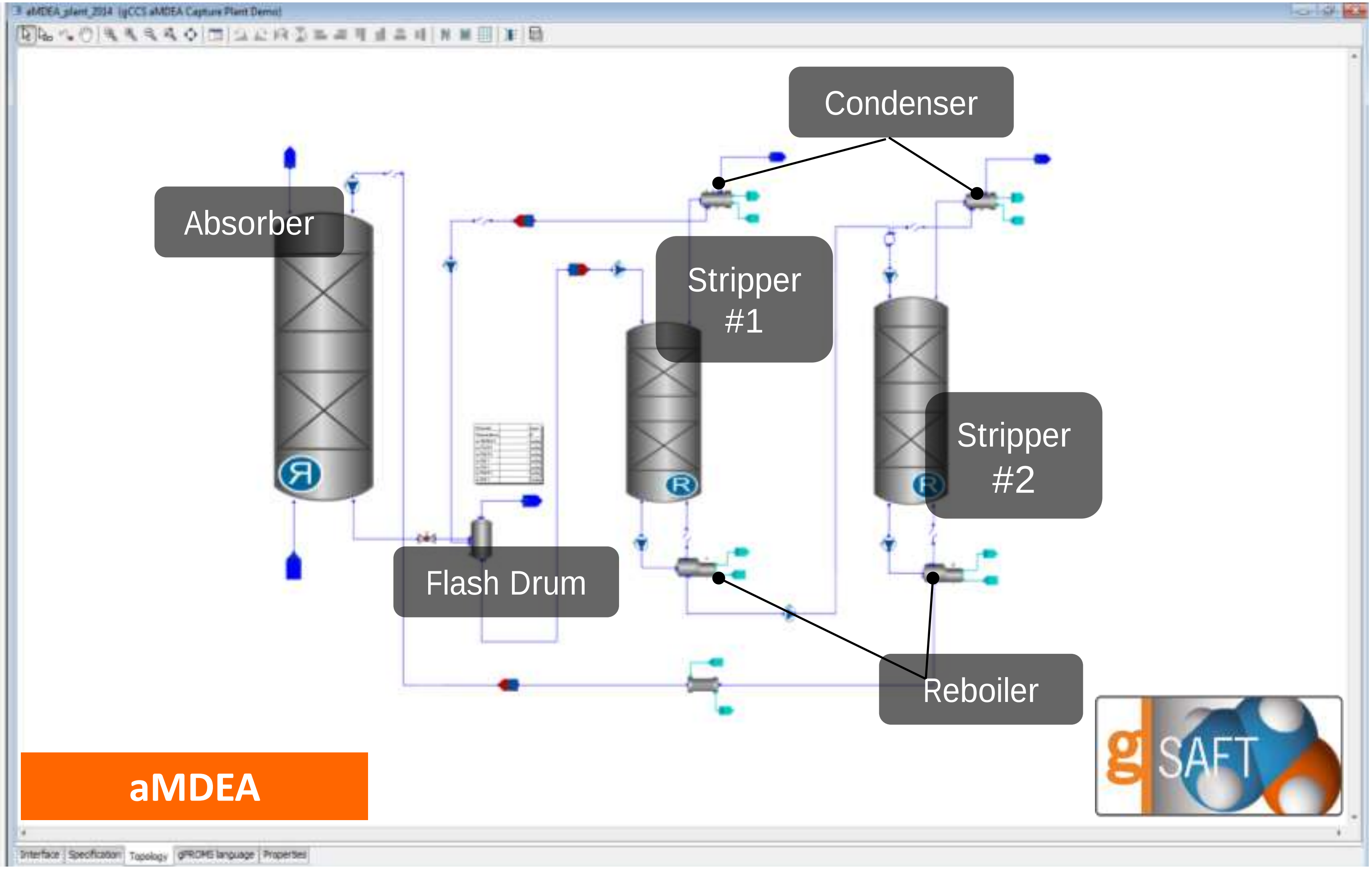


polyethylene glycol dimethyl ether (PEGDME)

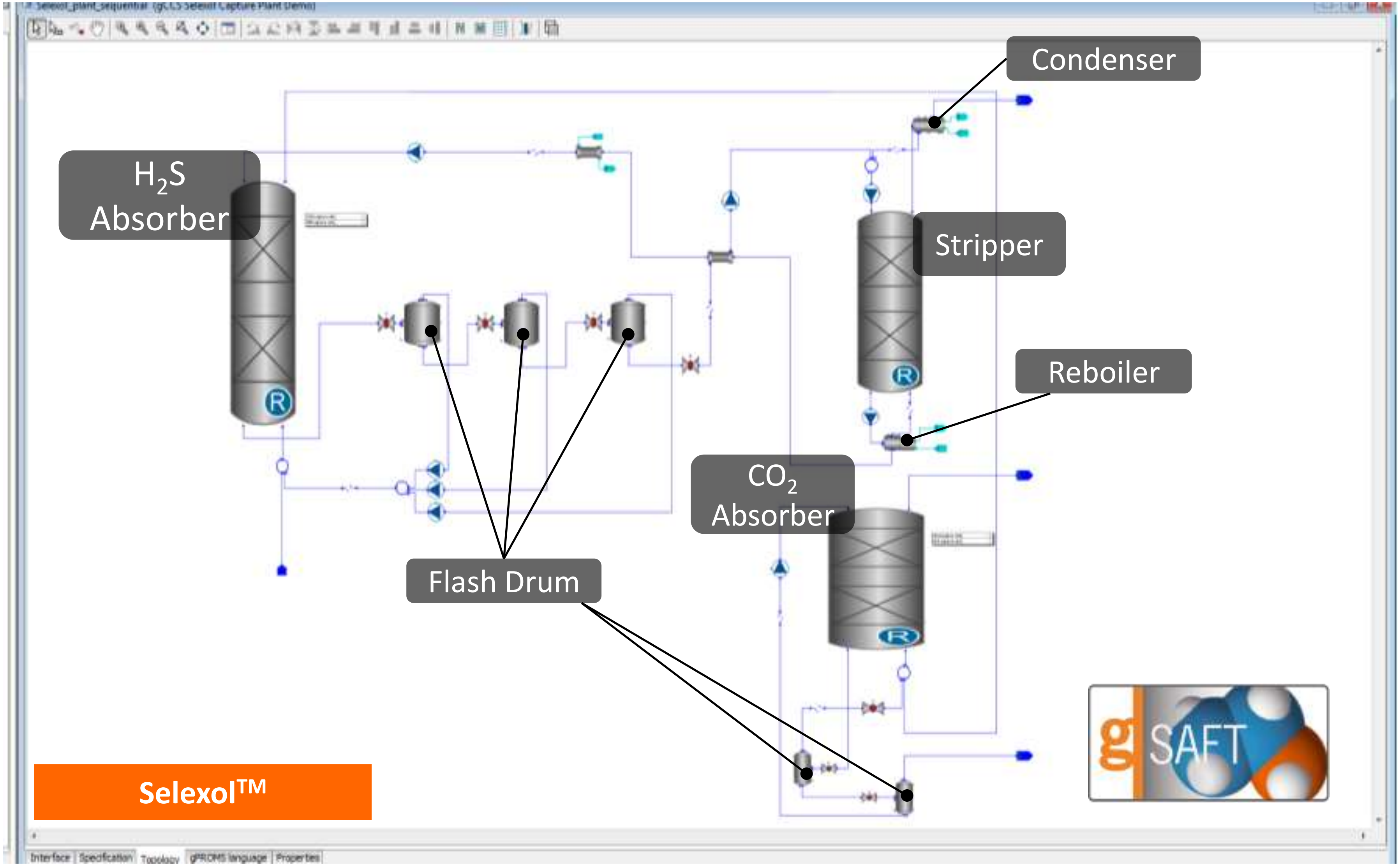
Material models for physical absorption



aMDEA process model



Selexol process model

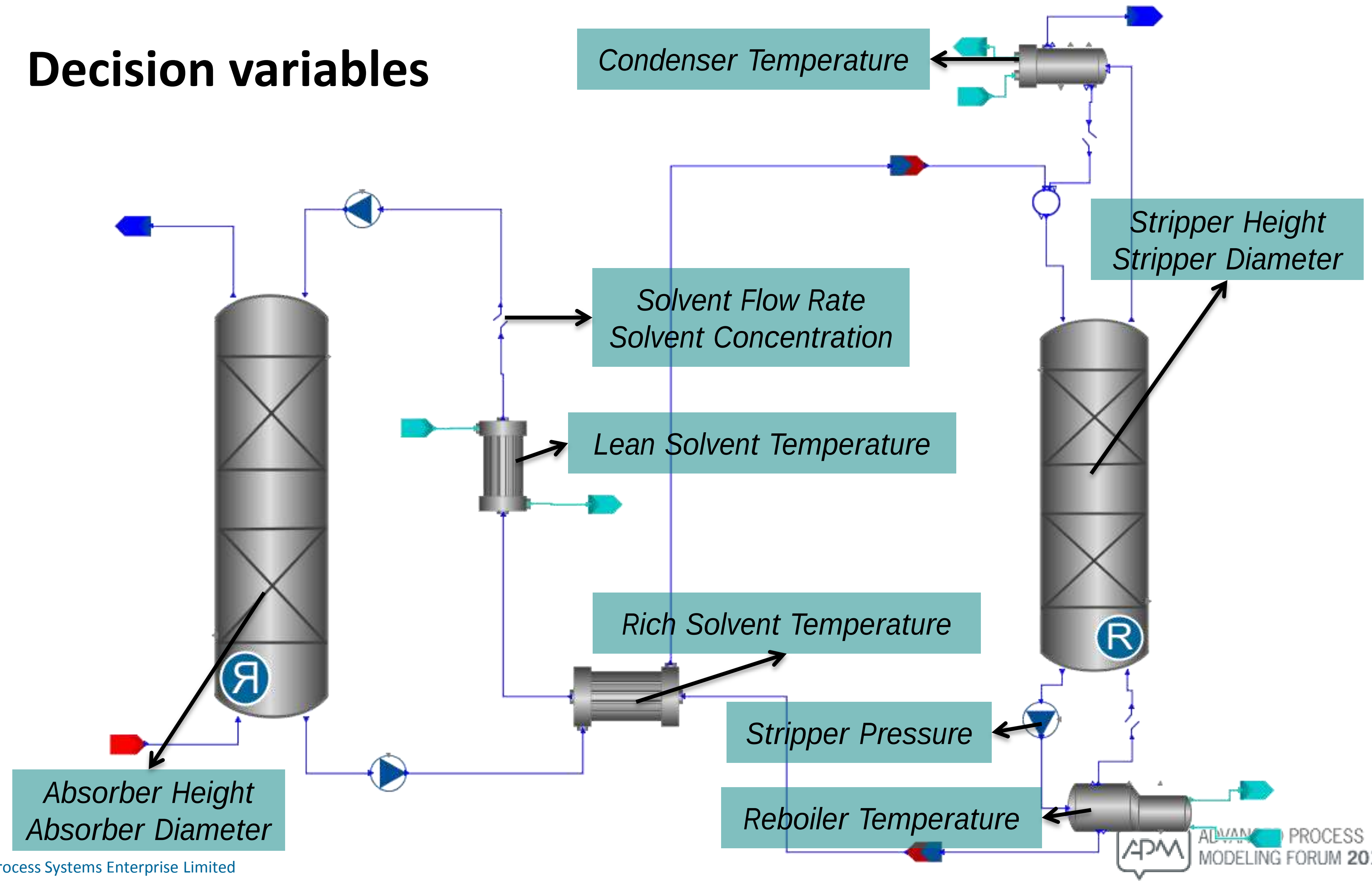


Process and solvent optimisation

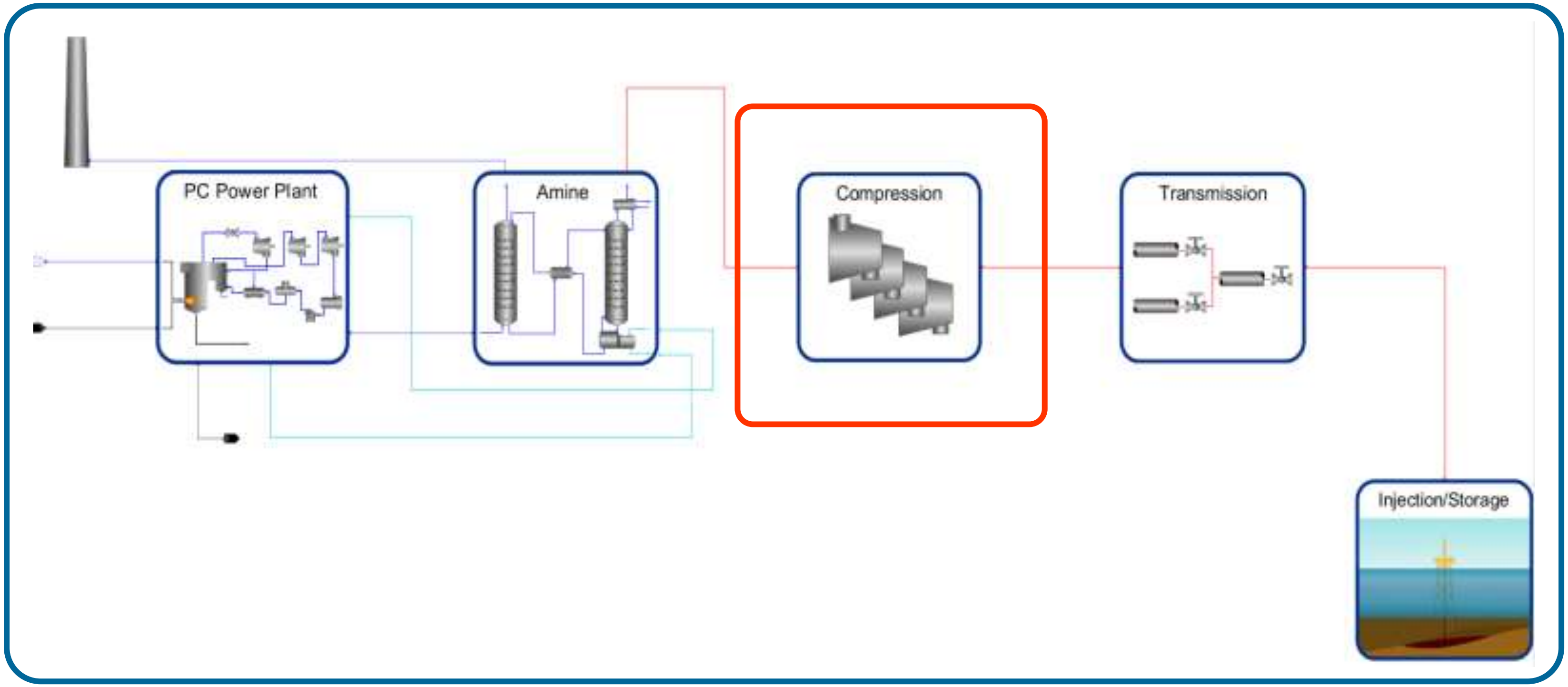
- gPROMS (equation-oriented) is well-suited to perform optimisation studies
  - Process
    - Plant configuration
    - Operating conditions
  - Solvent
    - Relative concentration of species
    - Solvent design: gSAFT is a group contribution method
- Case Study:
  - Process optimisation of a MEA pilot plant

Process and solvent optimisation

Decision variables

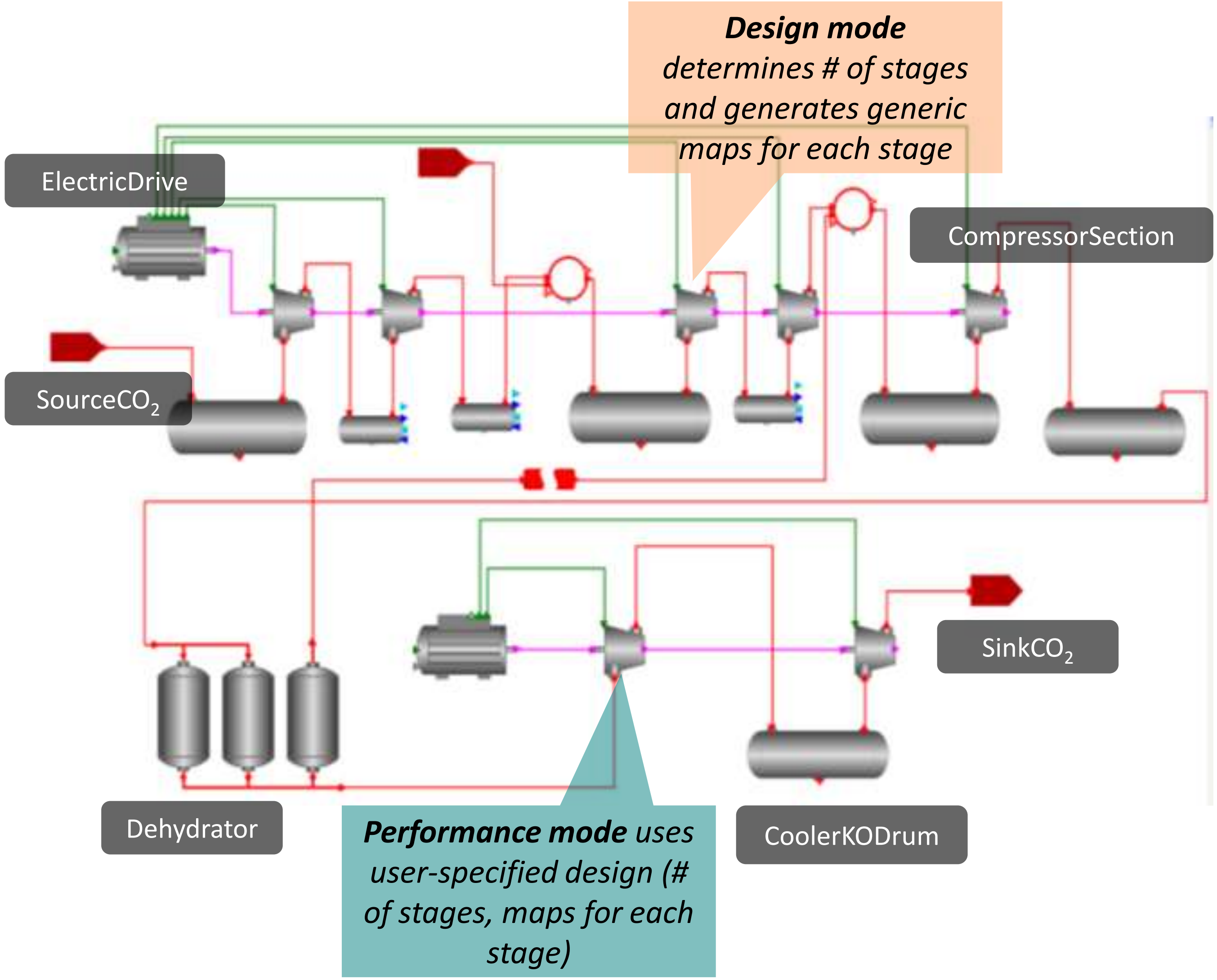


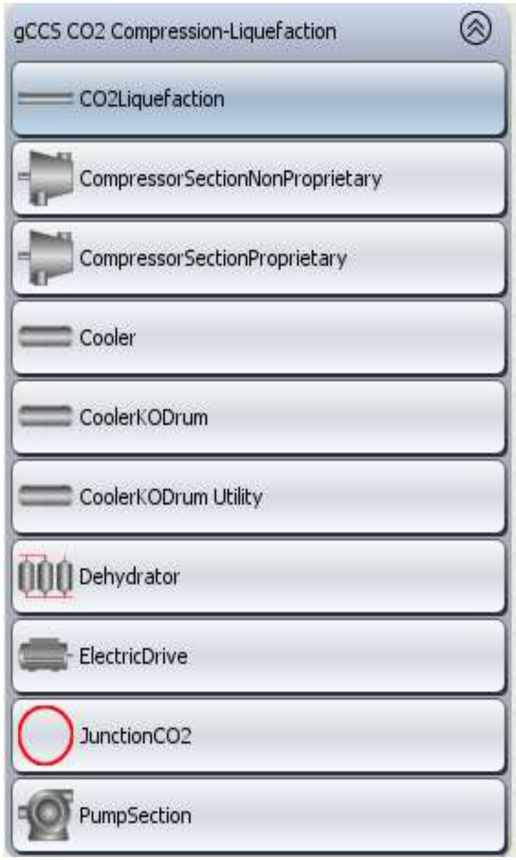
Compression



gCCS CO_2 Compression library

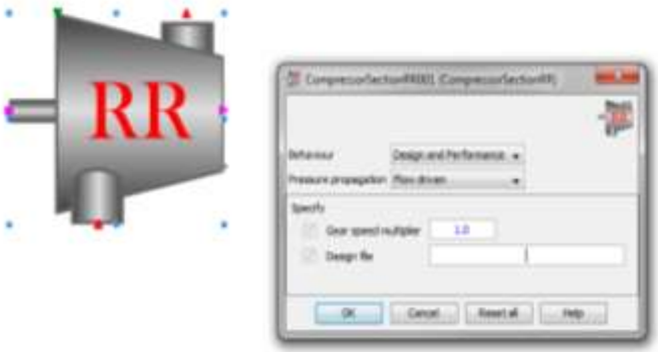
Compressor train components



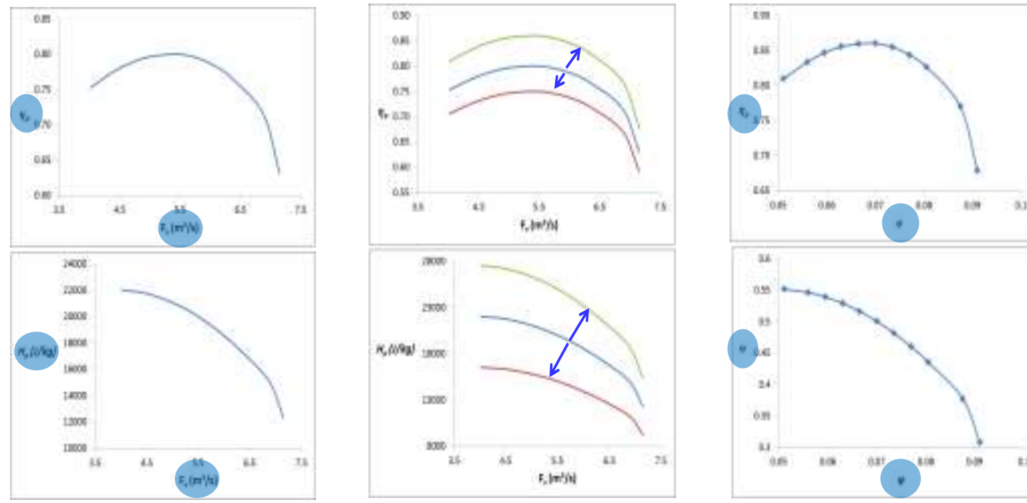


Key Features

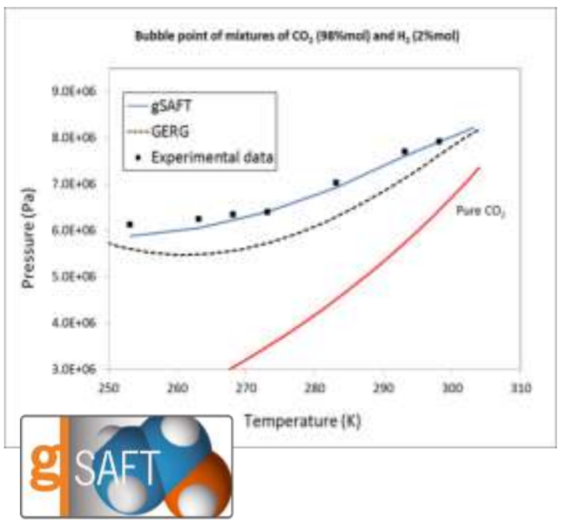
Interface with "in-house" tools



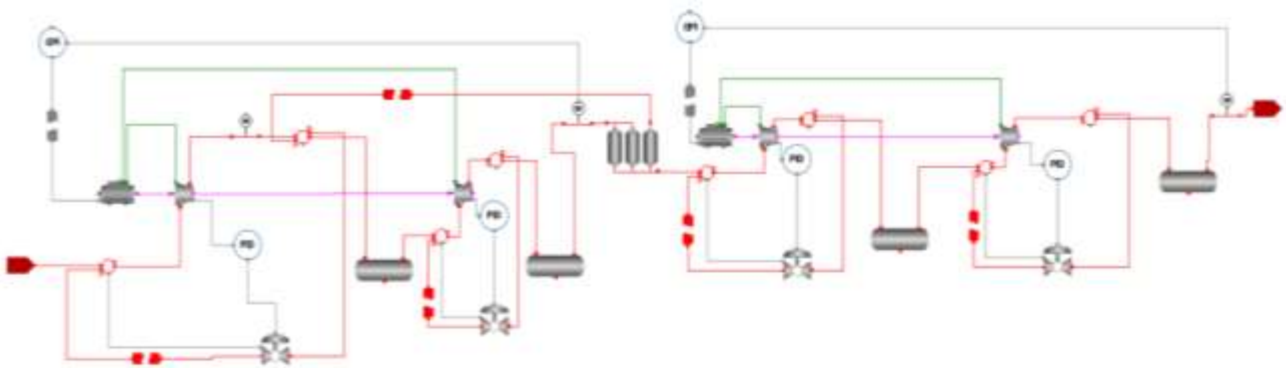
Performance map flexibility



Accurate physical properties



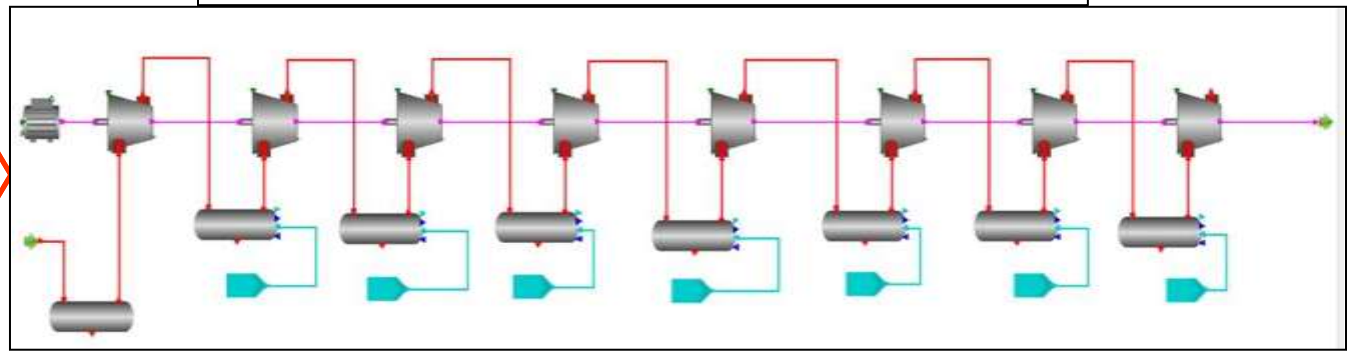
Surge and pressure control



Key Features

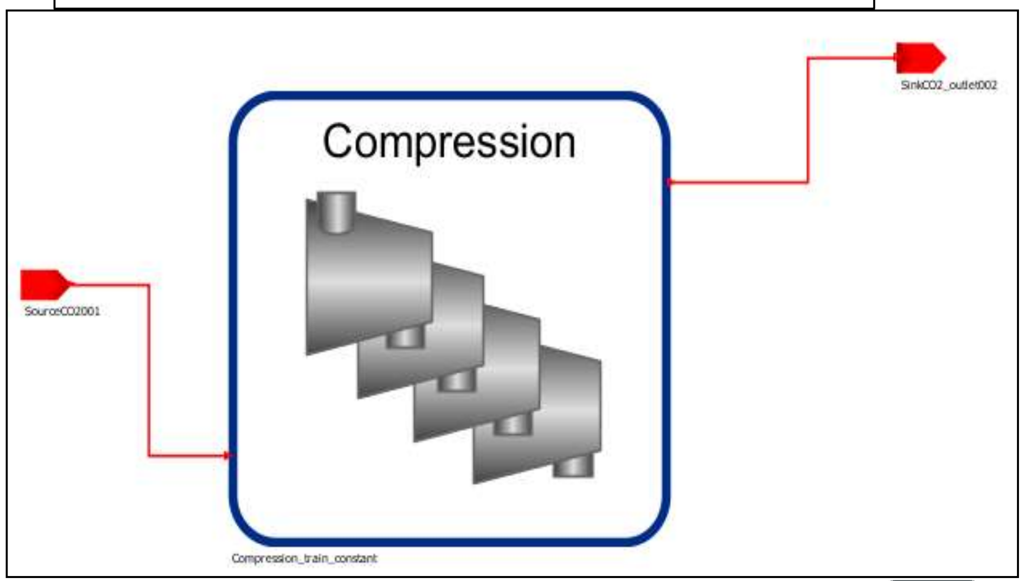
Tier I user
- R&D / Engineering
- "Modeller/Engineer"

Techno-economic mixed-integer optimisation

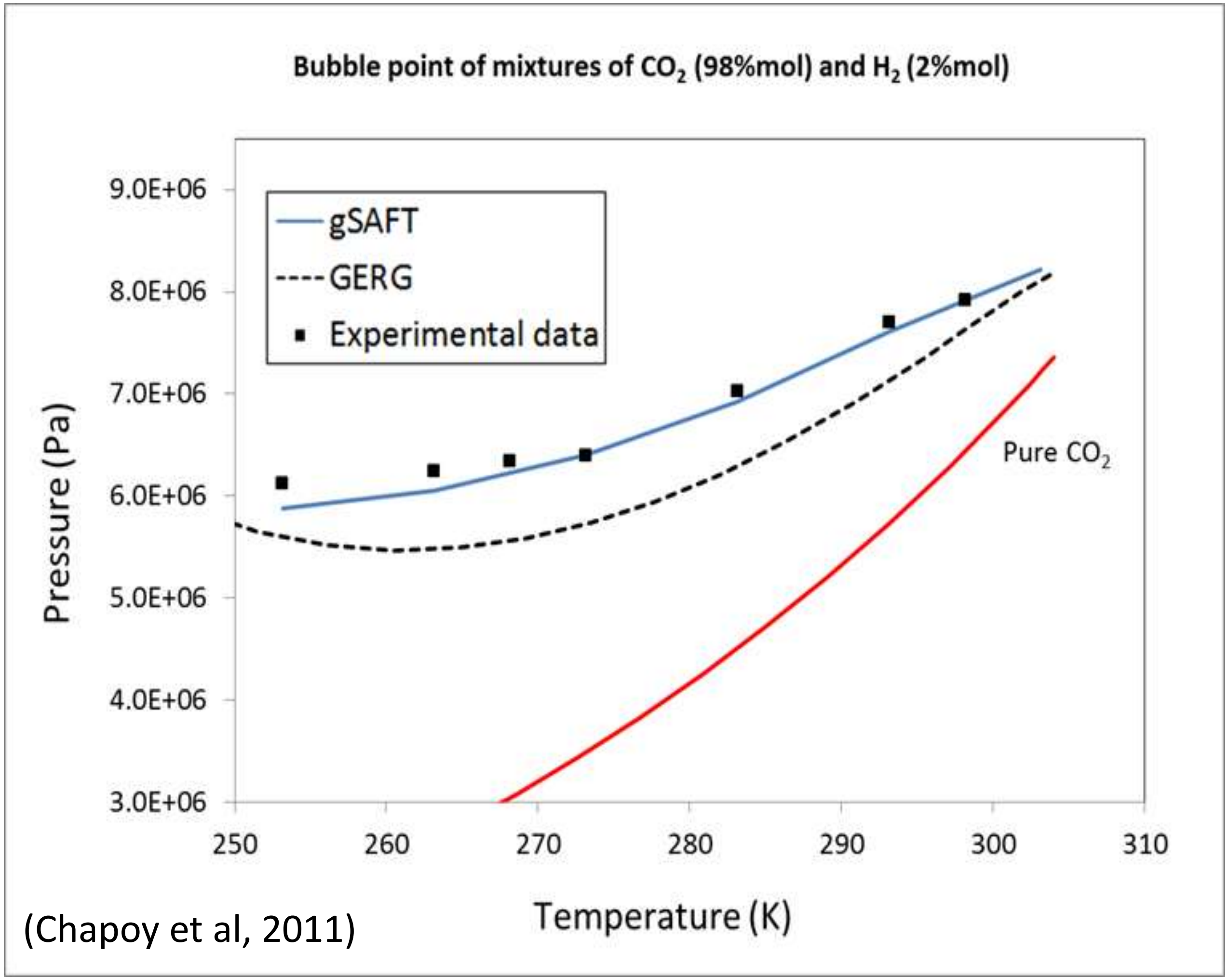


Tier III user
- Engineering / Commercial
- "Decision/Policy maker"

High-level compression train model

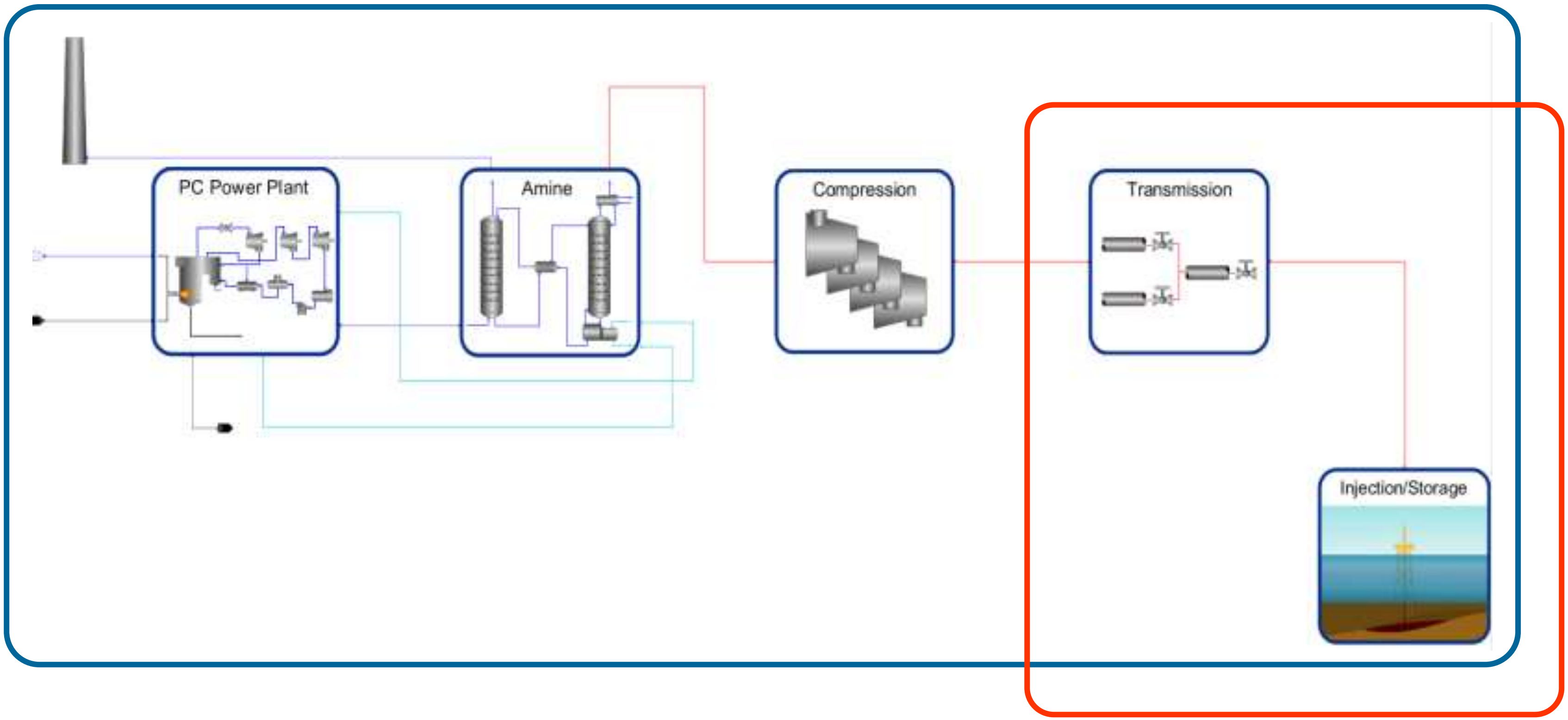


Binary mixture of H_2 and CO_2



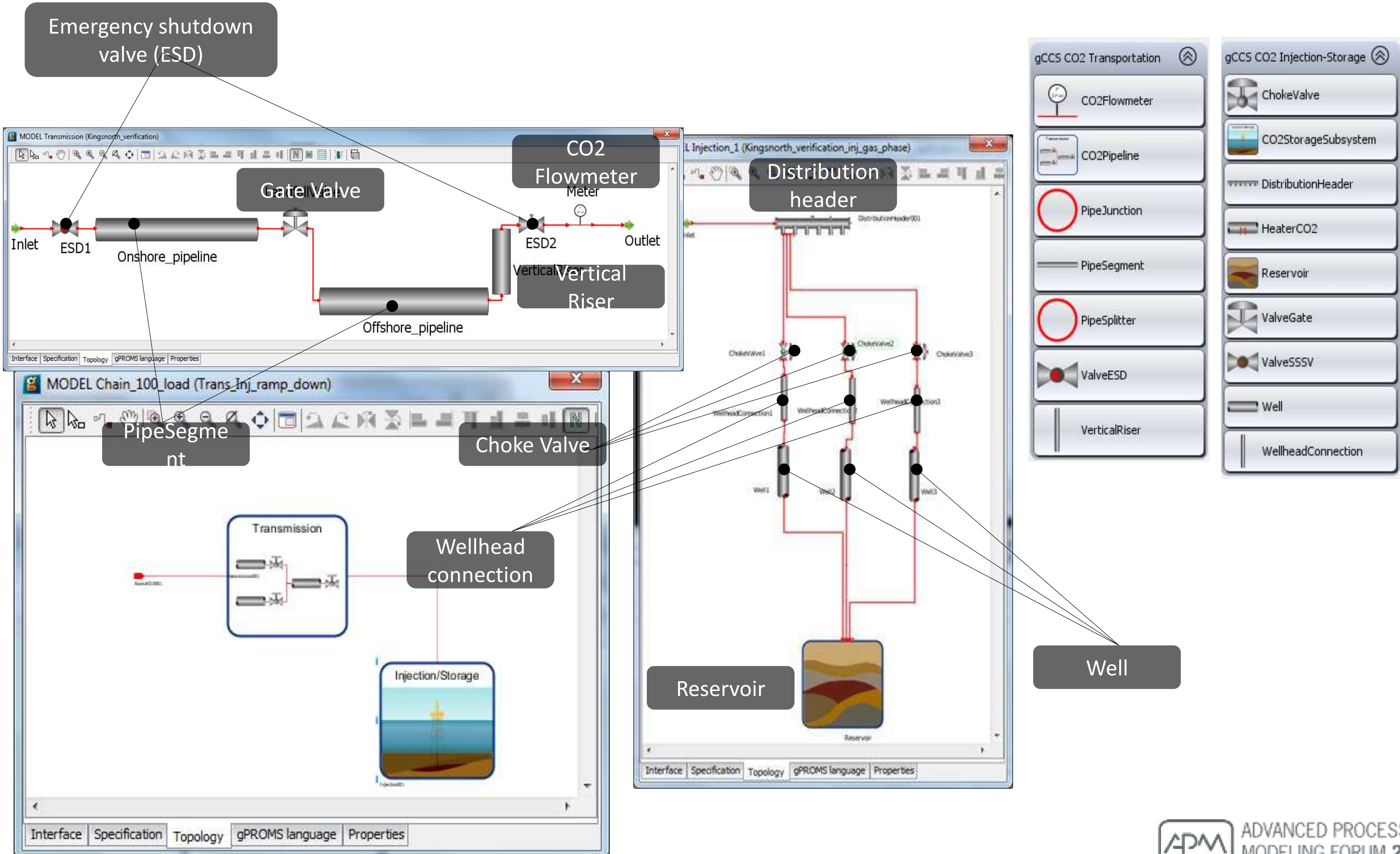
(Chapoy et al, 2011)

Transmission & injection



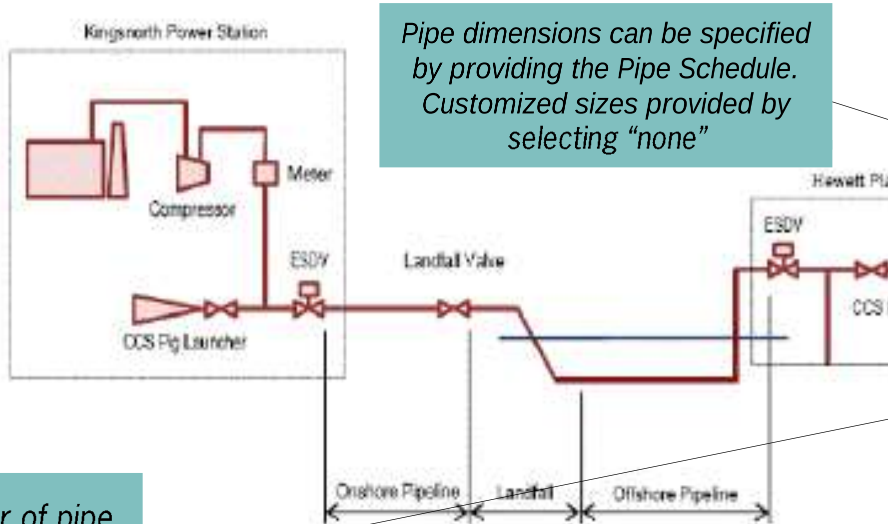
gCCS Transmission & Injection/Storage

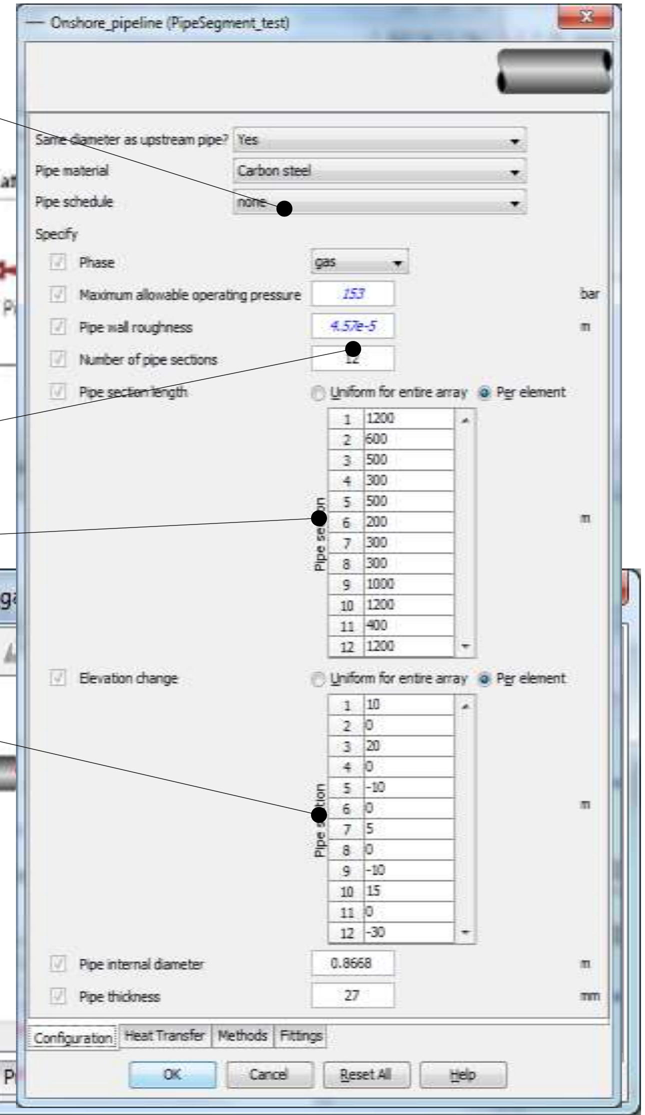
Features

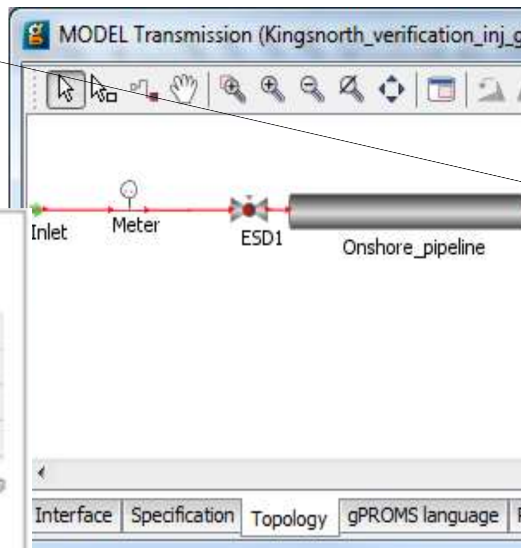


Features

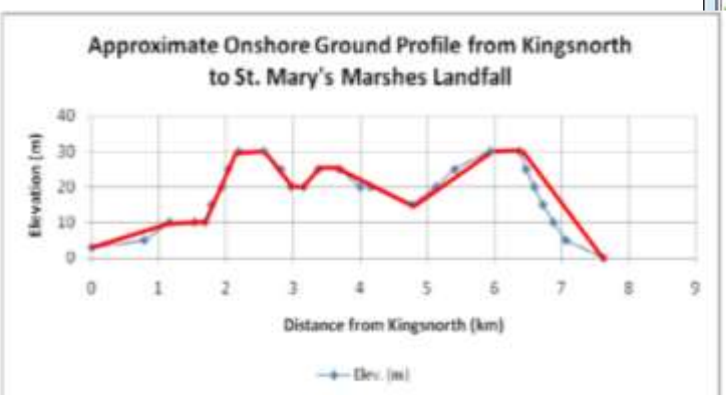
Pipe dimensions can be specified by providing the Pipe Schedule. Customized sizes provided by selecting "none"



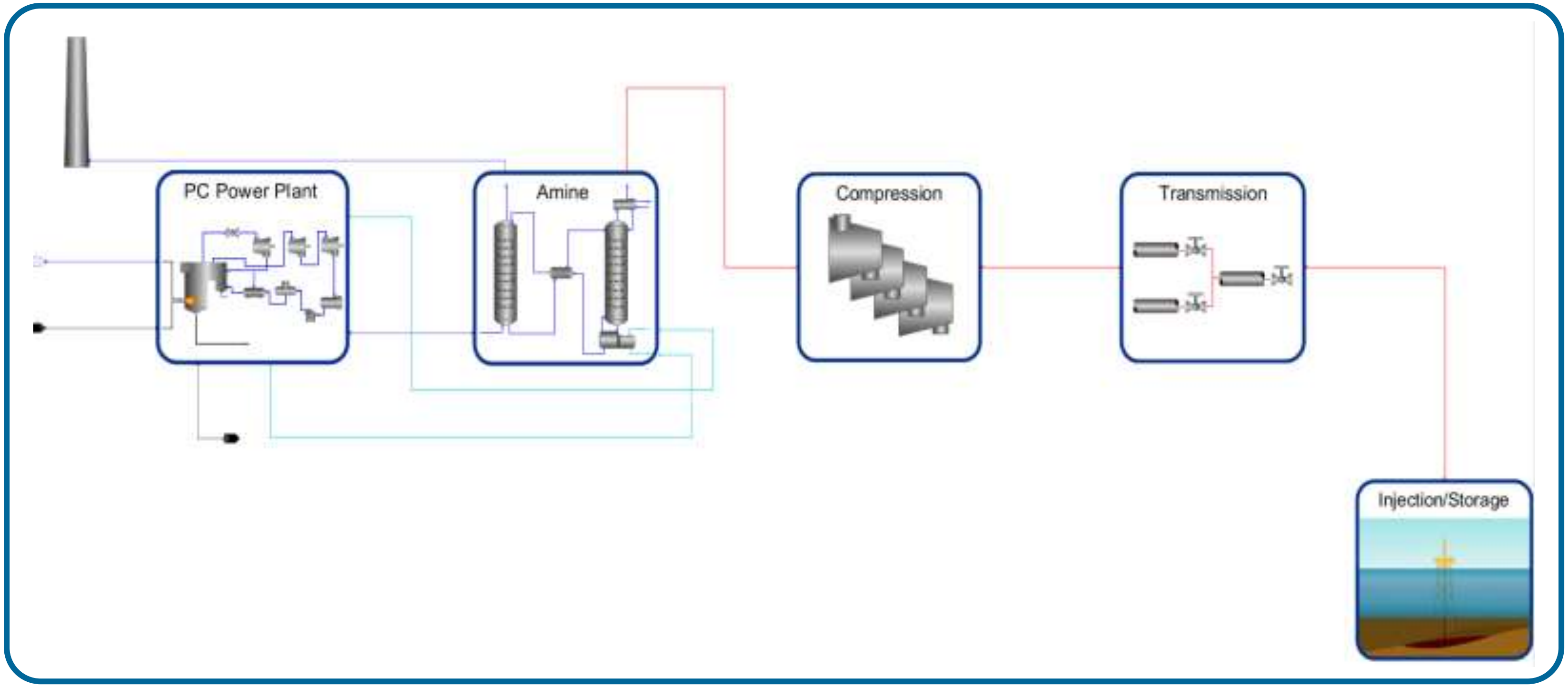




The value of "Number of pipe sections" determines the number of "Pipe section" fields

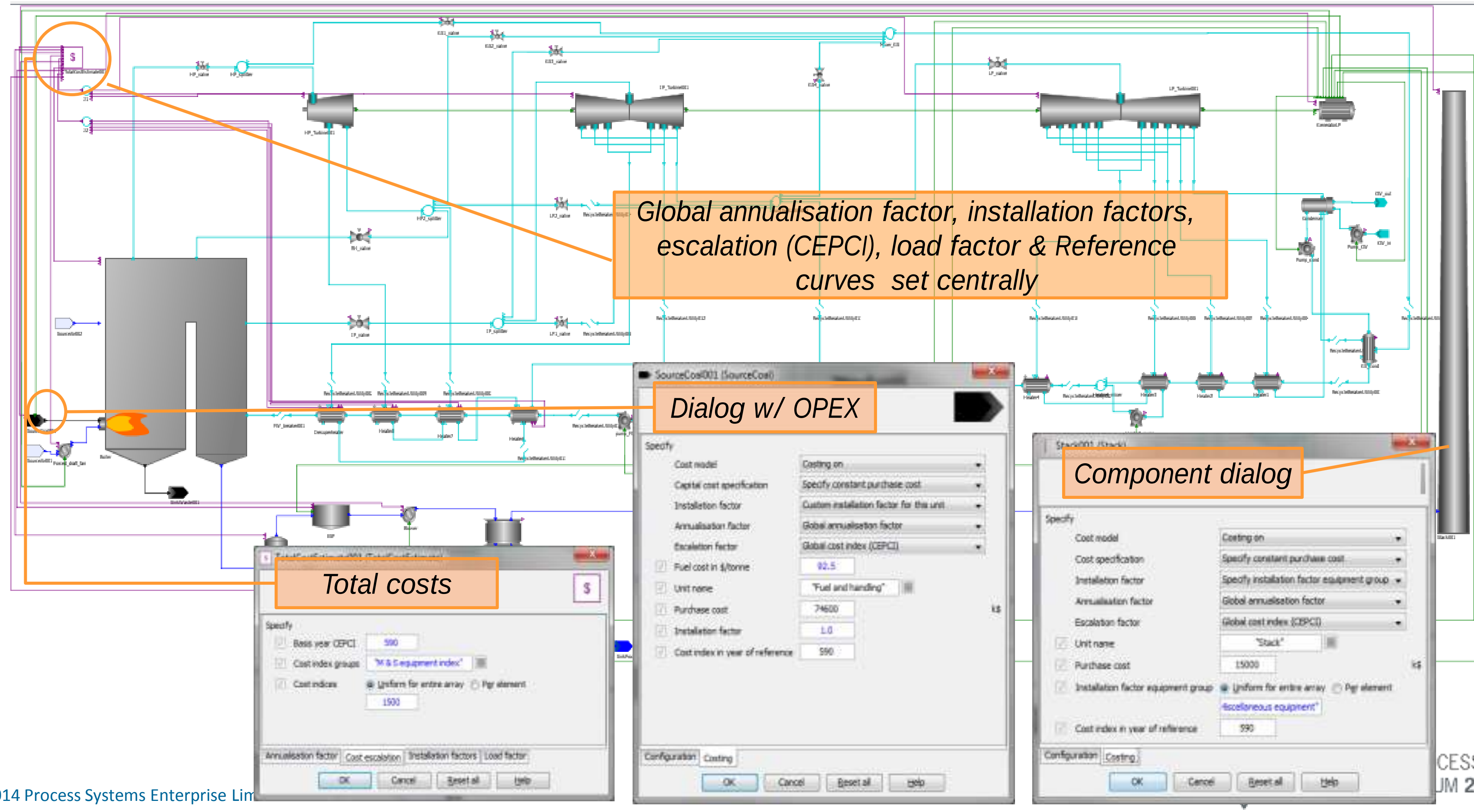


Whole chain capabilities



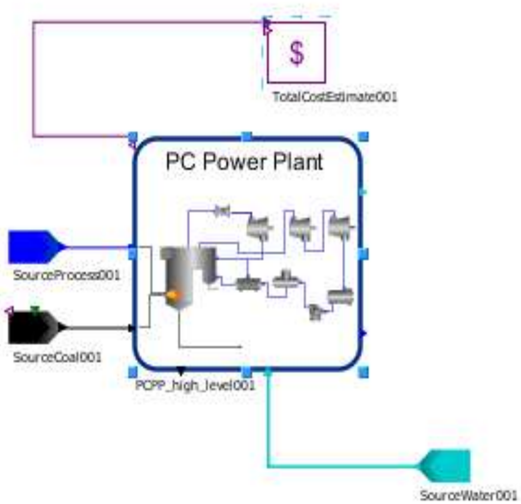
Costing

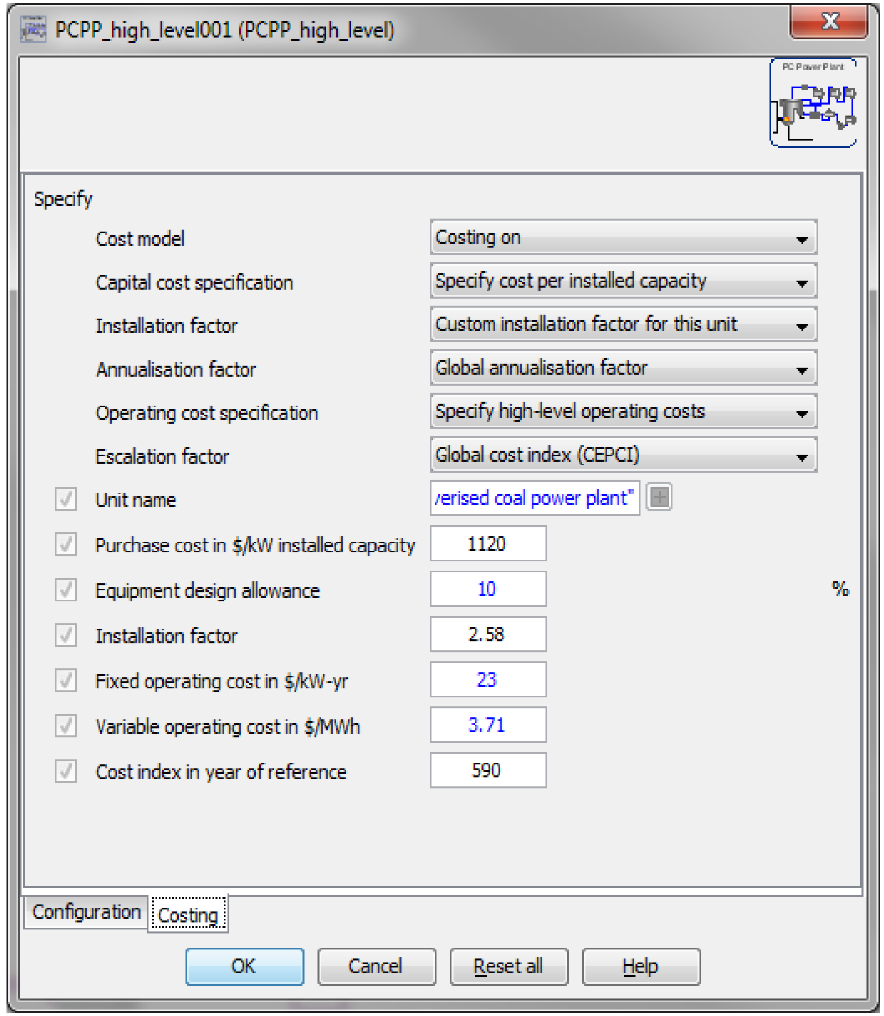
- Component costs configured within the unit – fixed purchase cost or power curve with relevant sizing value calculated by the model



High level sub-system models

- High level models:
  - High level costing
  - CAPEX per installed kW
  - Fixed & Variable OPEX



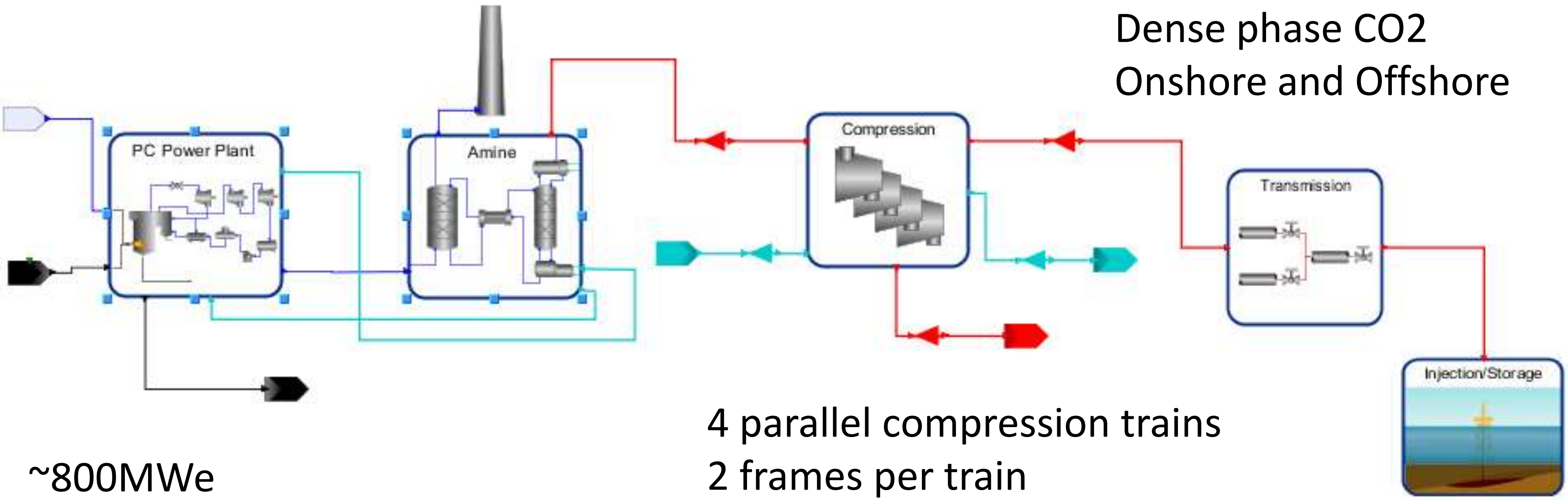


Case Study: CCS chain

System overview

Chemical absorption
MEA solvent
90% CO_2 capture

220km pipeline
Dense phase CO2
Onshore and Offshore

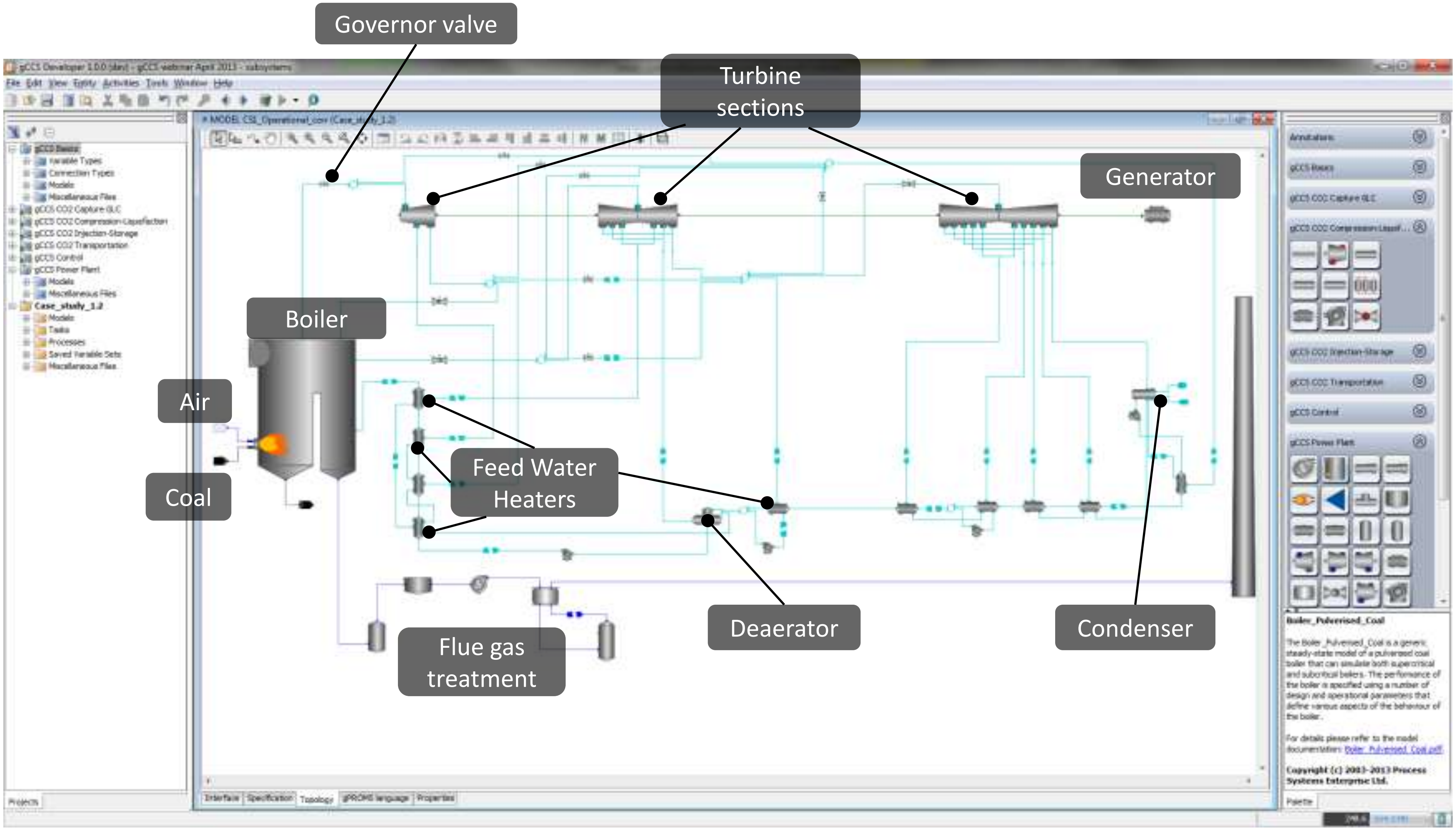


~800MWe
Supercritical
Pulverized coal
(acknowledgement: E.ON)

4 parallel compression trains
2 frames per train
Surge control
(acknowledgement:
Rolls-Royce)

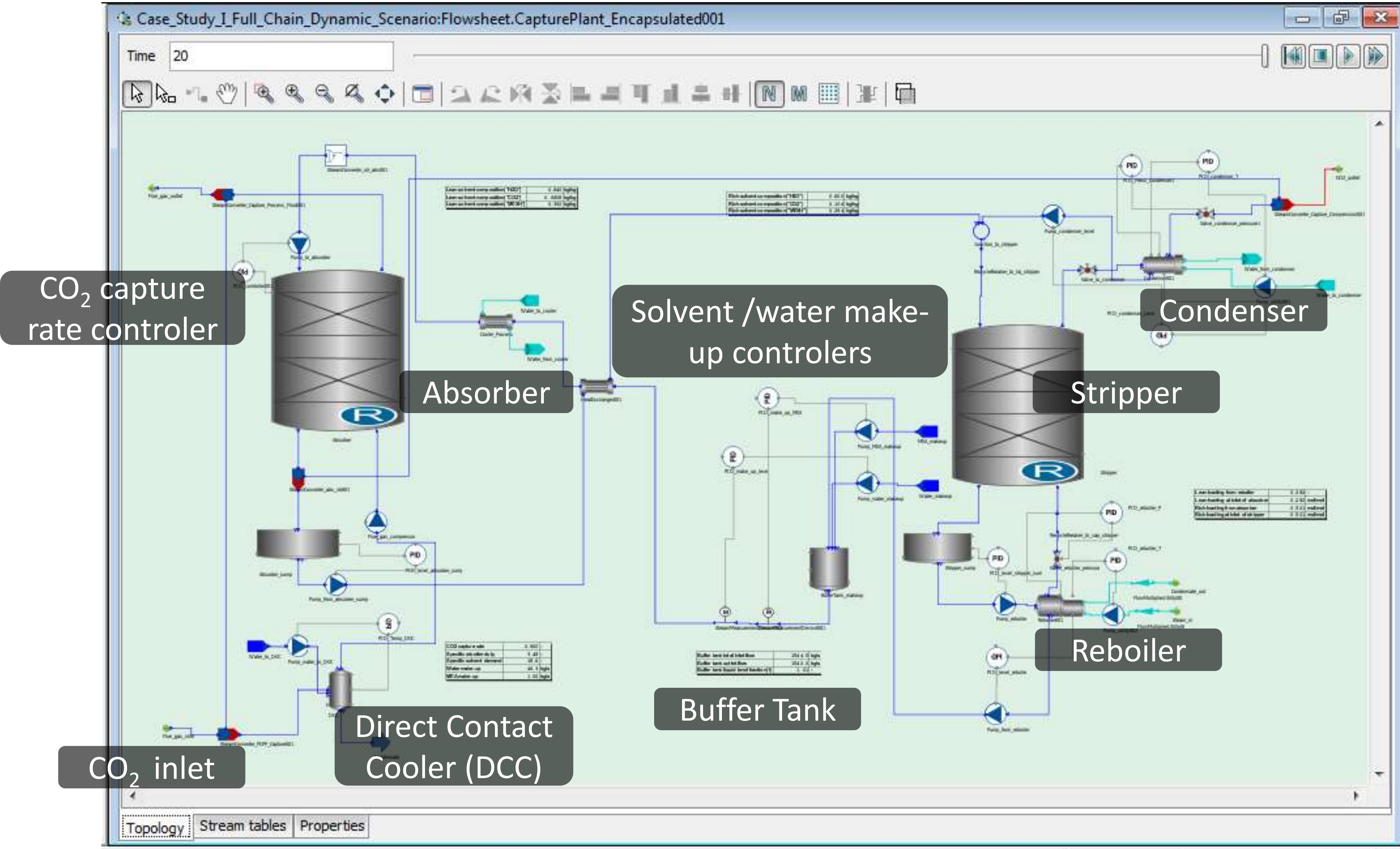
Offshore dense-phase
injection; 4 injection wells
~2km reservoir depth
(acknowledgement:
CO2DeepStore)

Supercritical pulverized coal power plant



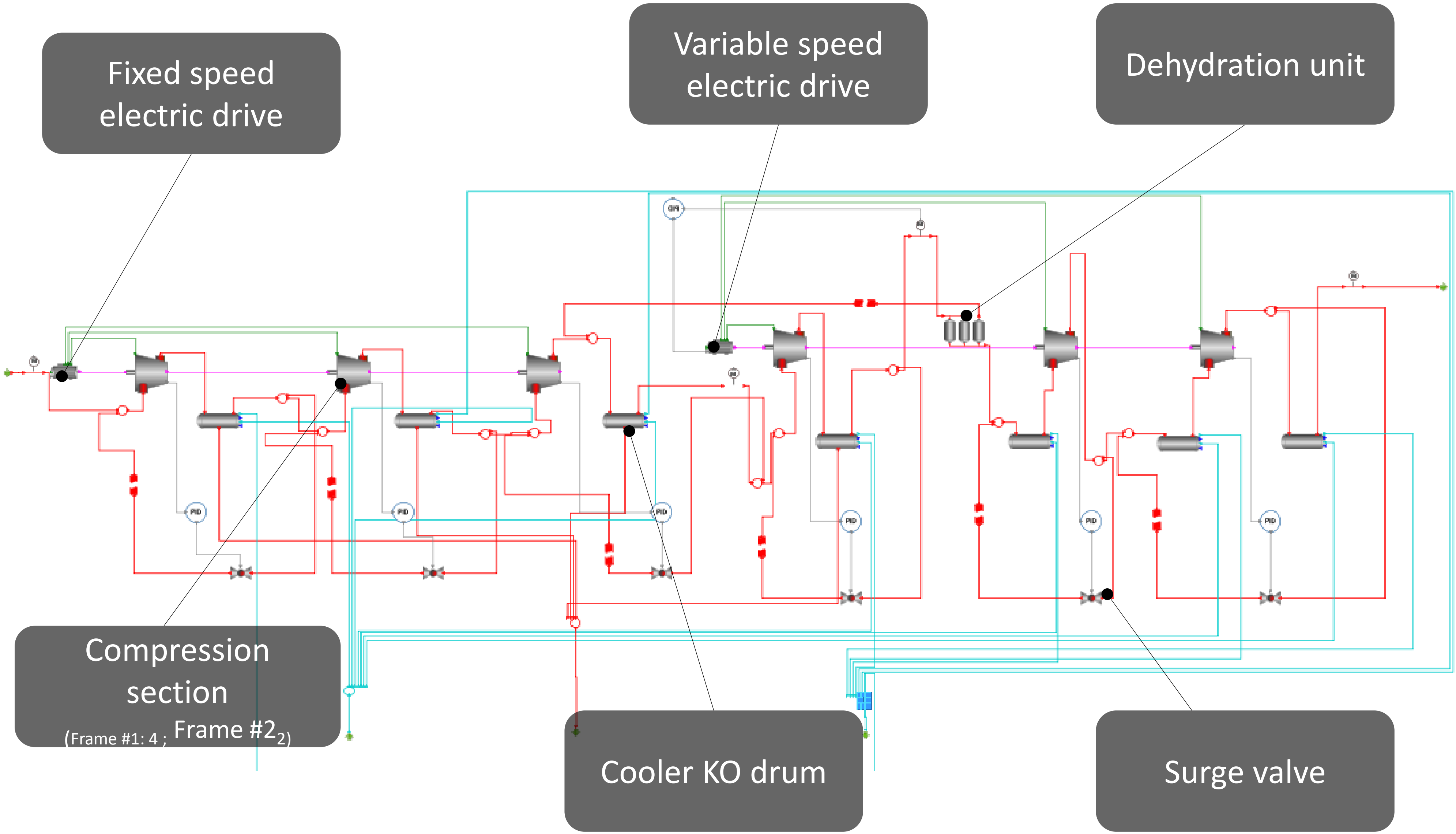
Sub-system #2

CO_2 capture plant



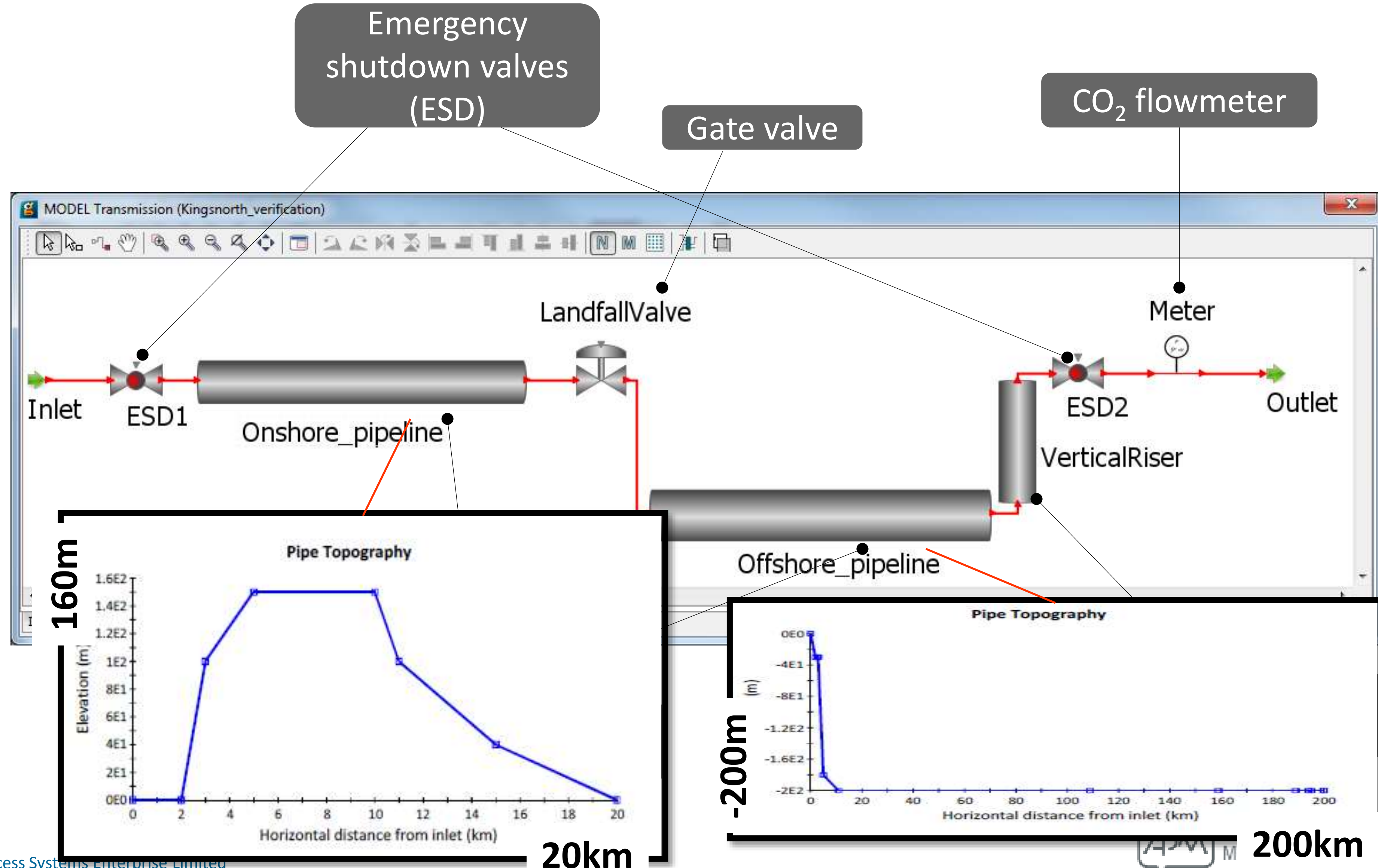
Sub-system #3

CO_2 compression plant



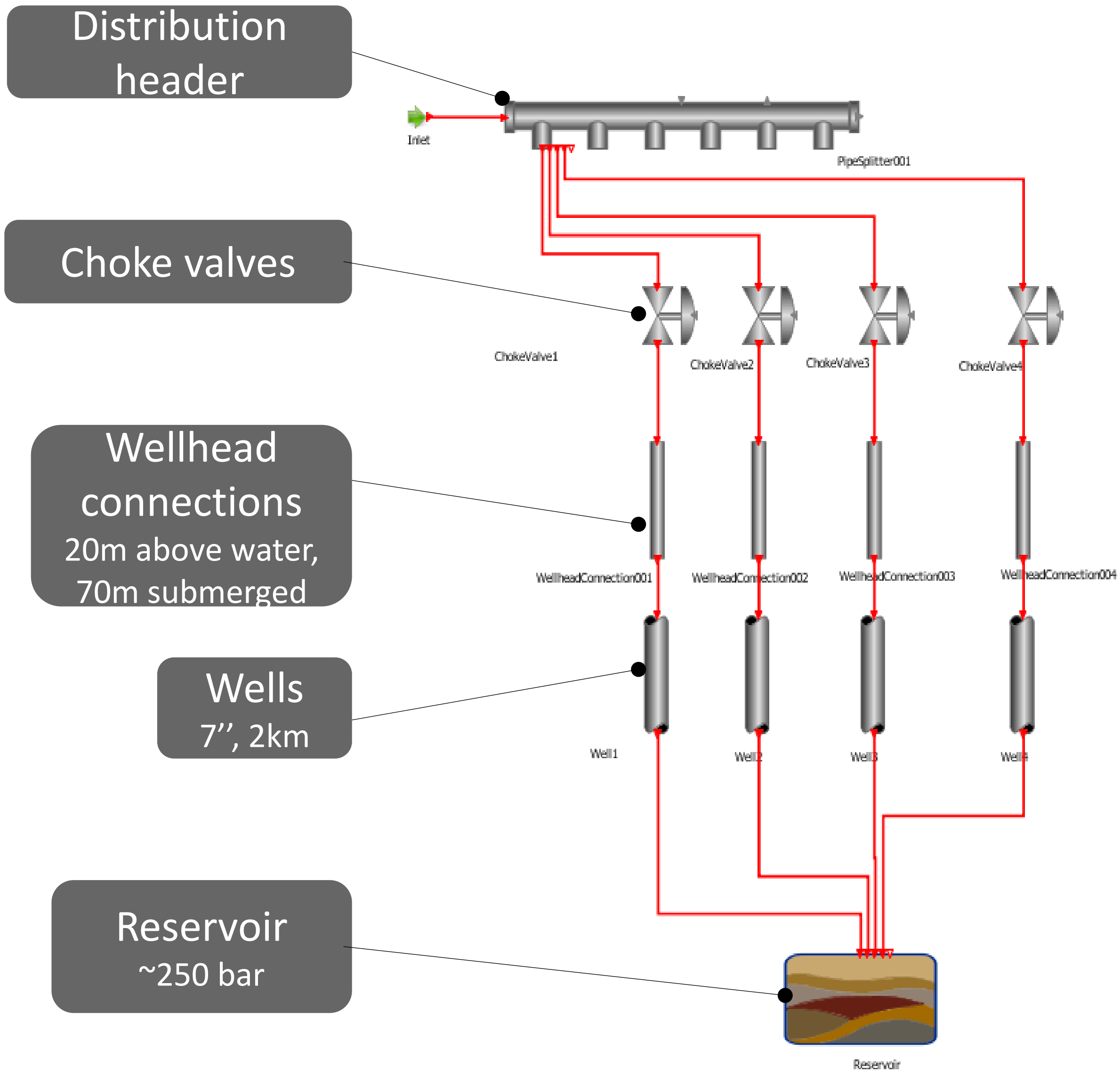
Sub-system #4

CO_2 transmission pipelines



Sub-system #5

CO_2 injection & storage in reservoir



Case Study: dynamic analysis

Single CCS Chain

Why dynamic analysis?

– Inflexible intermittent generation (e.g. wind & solar) means fossil fuel plants will be required to change load around less predictable changes in green supply

Case Study

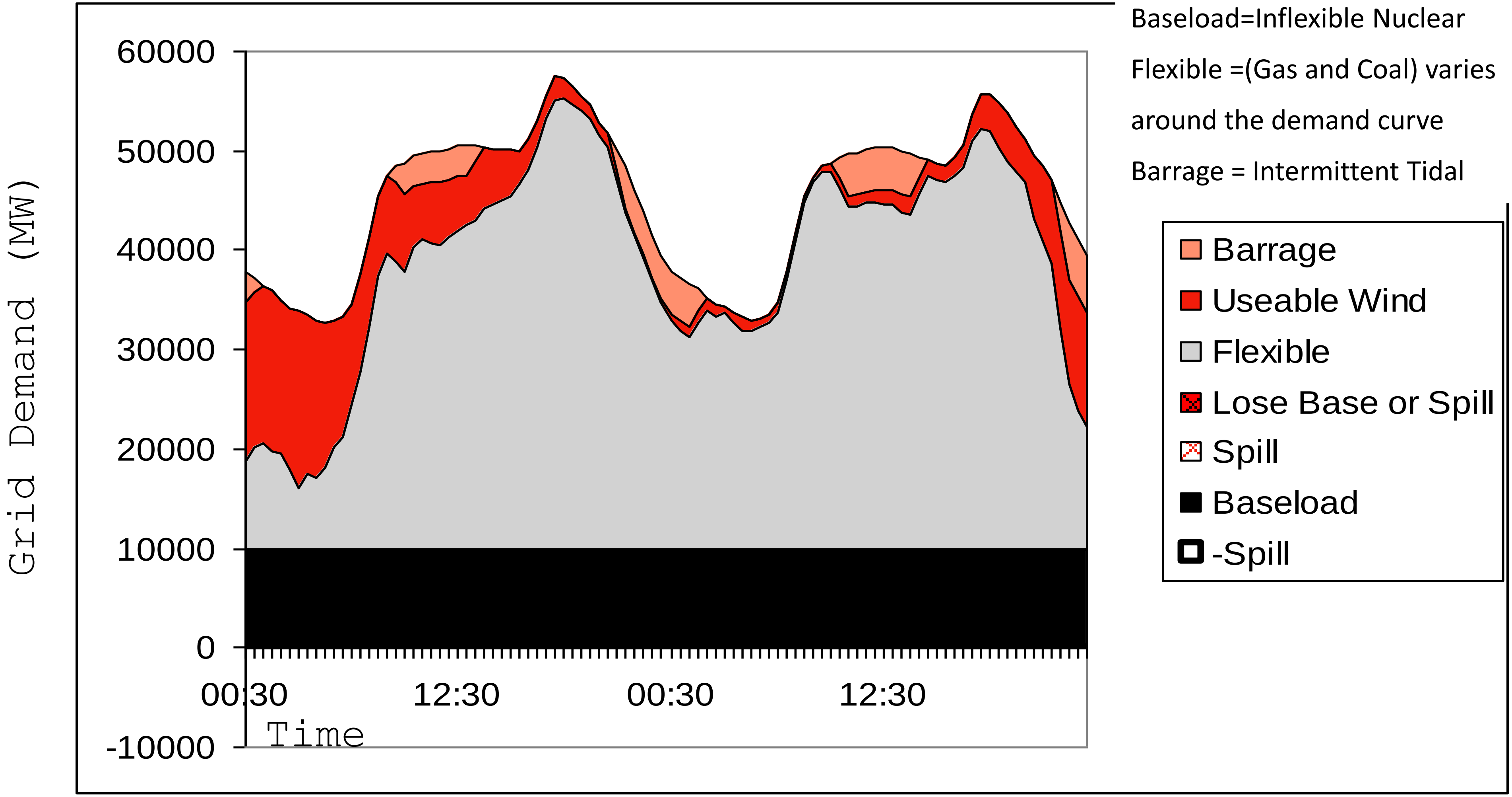
Typical day in 2010

Wind= low penetration

Baseload=Inflexible Nuclear

Flexible =(Gas and Coal) varies around the demand curve

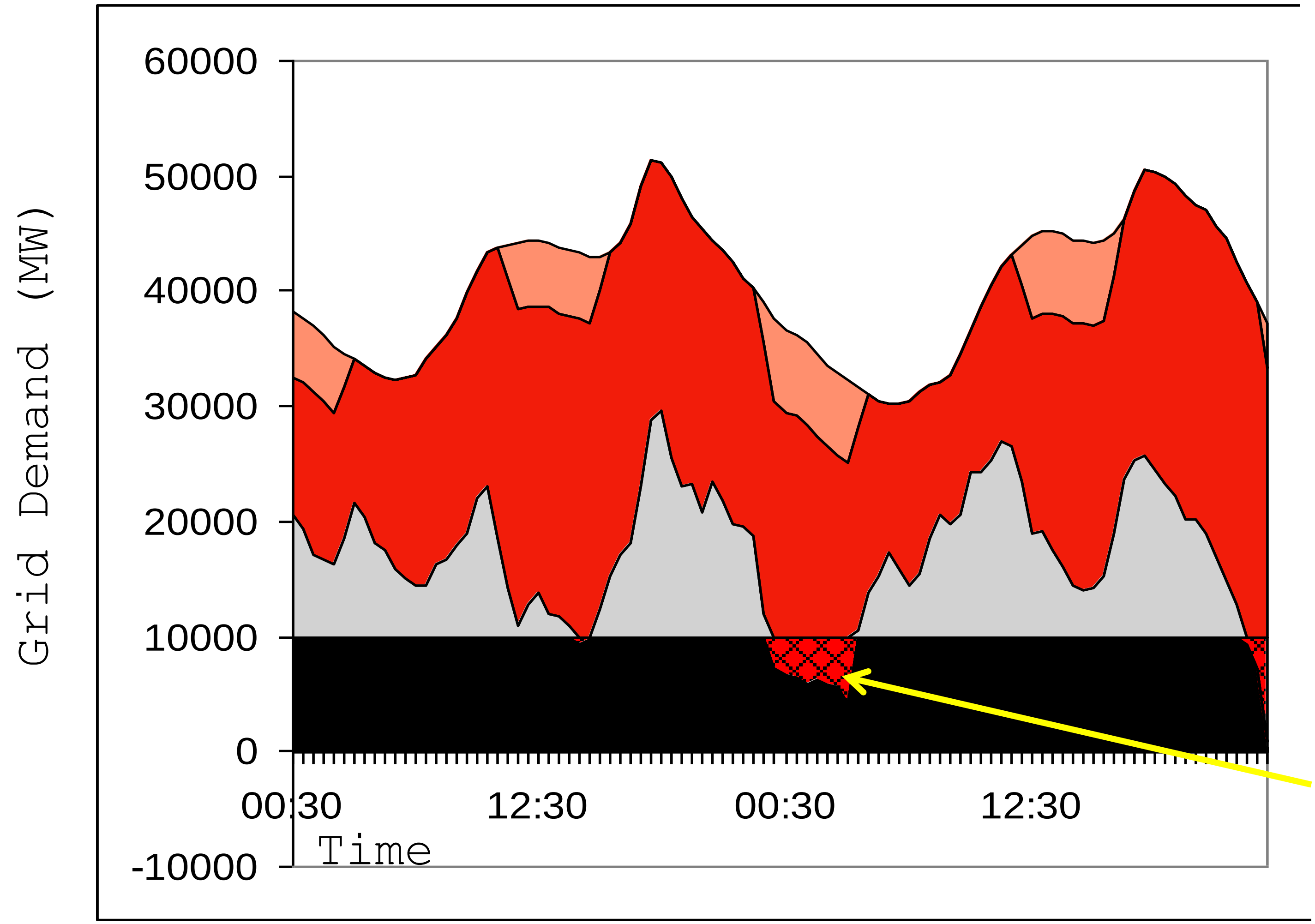
Barrage = Intermittent Tidal



Source: e·on

Case Study

Windy day in 2030 with high wind penetration



Wind= high penetration

Flexible =(Gas and Coal) varies around the demand curve and also variations in wind power

Additional power at night is large enough to impact base load plant – requires spill of renewable or baseload power.

Source: e·on

Single CCS Chain

Why dynamic analysis?

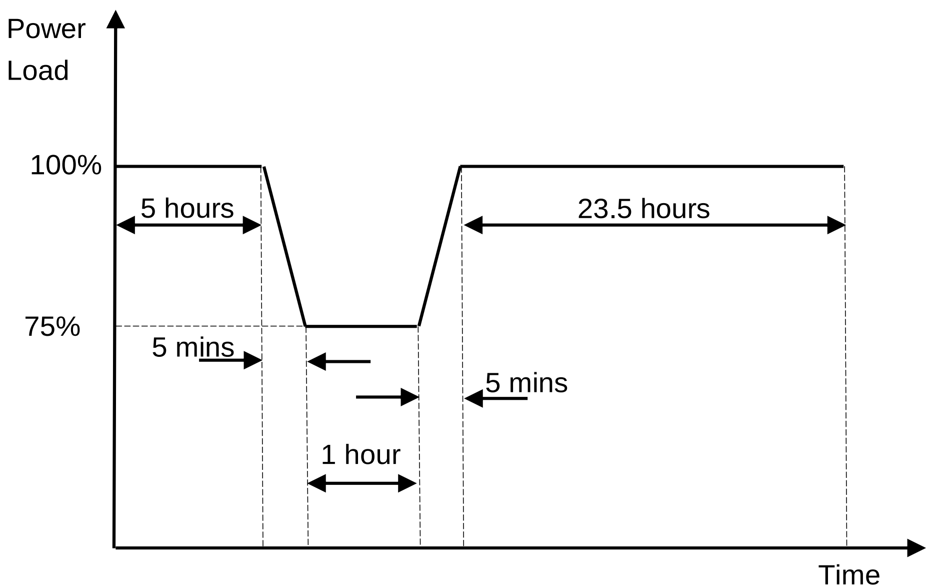
- Inflexible intermittent generation (e.g. wind & solar) means fossil fuel plants will be required to change load around less predictable changes in green supply

- However, capture plants normally operated at steady-state in traditional gas sweetening operations

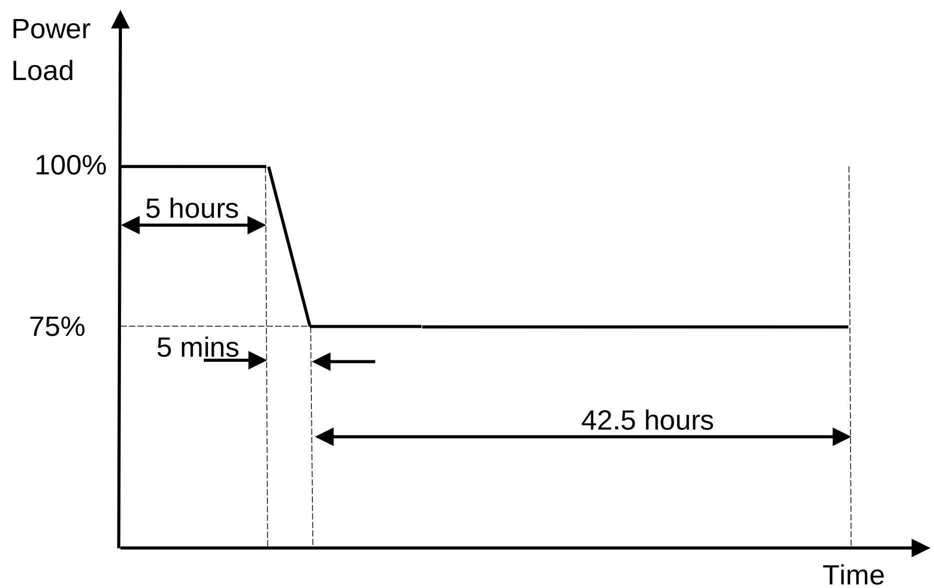
- Therefore, flexible operation of large-scale integrated CCS projects needs to be proven

Scheduled changes in power plant load

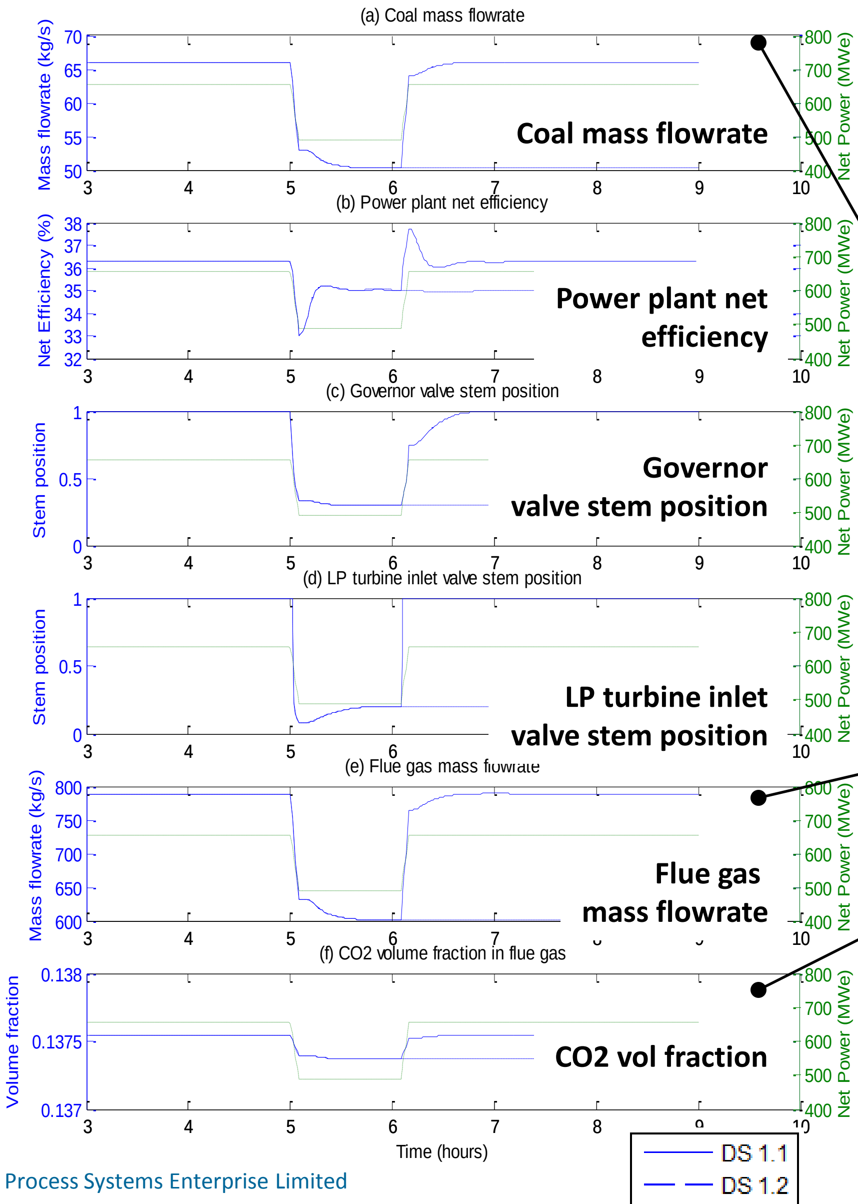
Scenario DS1.1

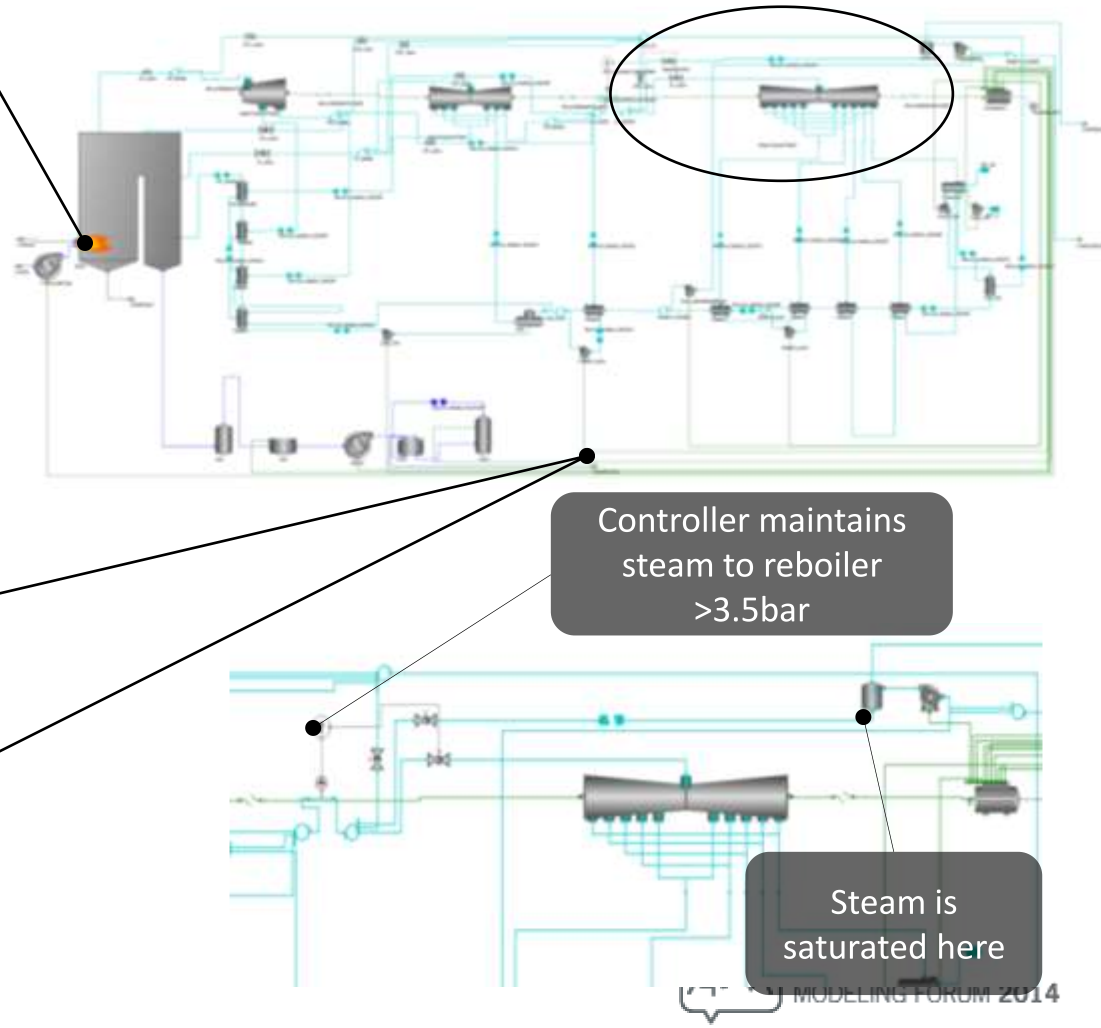


Scenario DS1.2



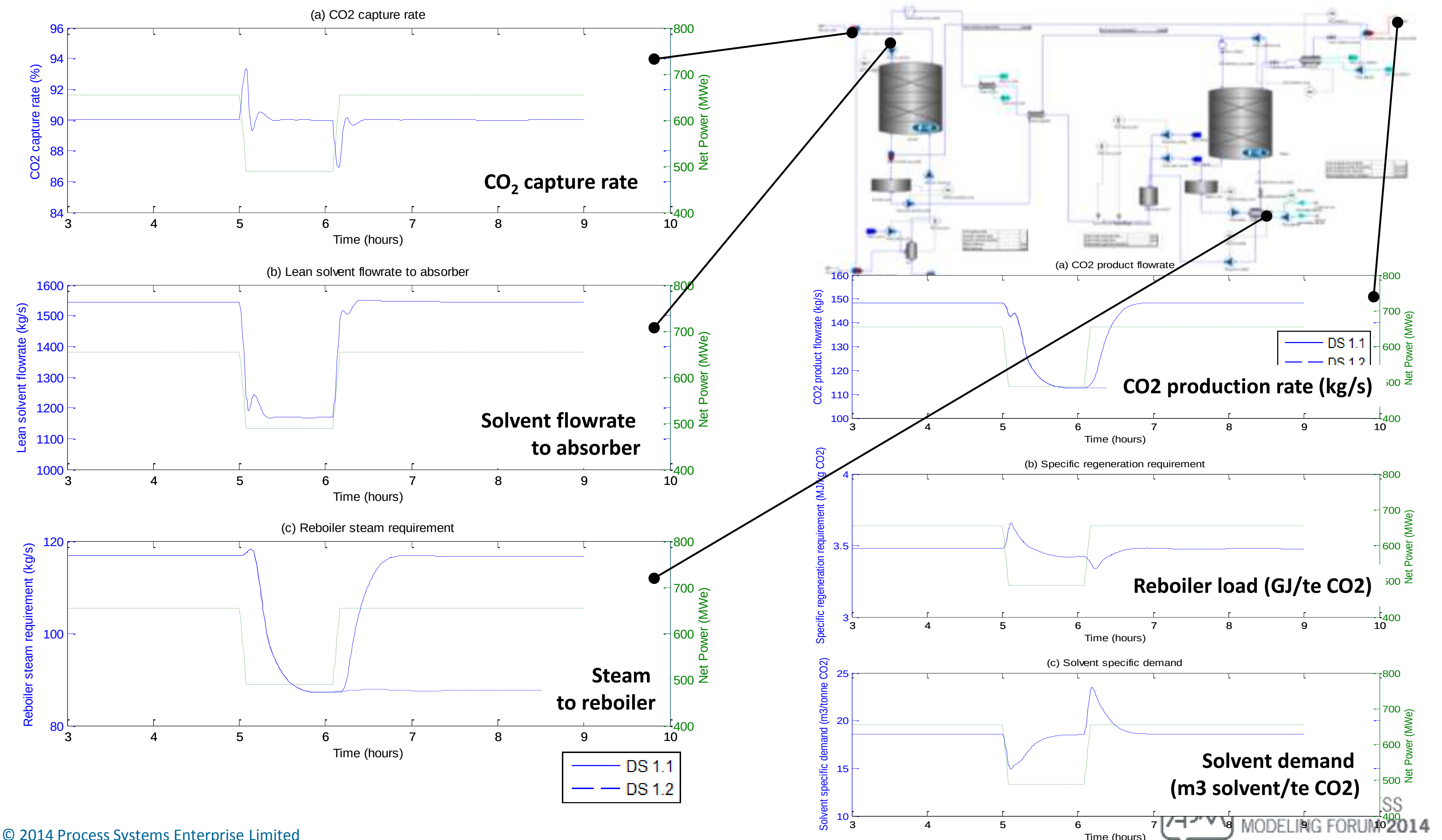
Dynamic analysis
Power plant



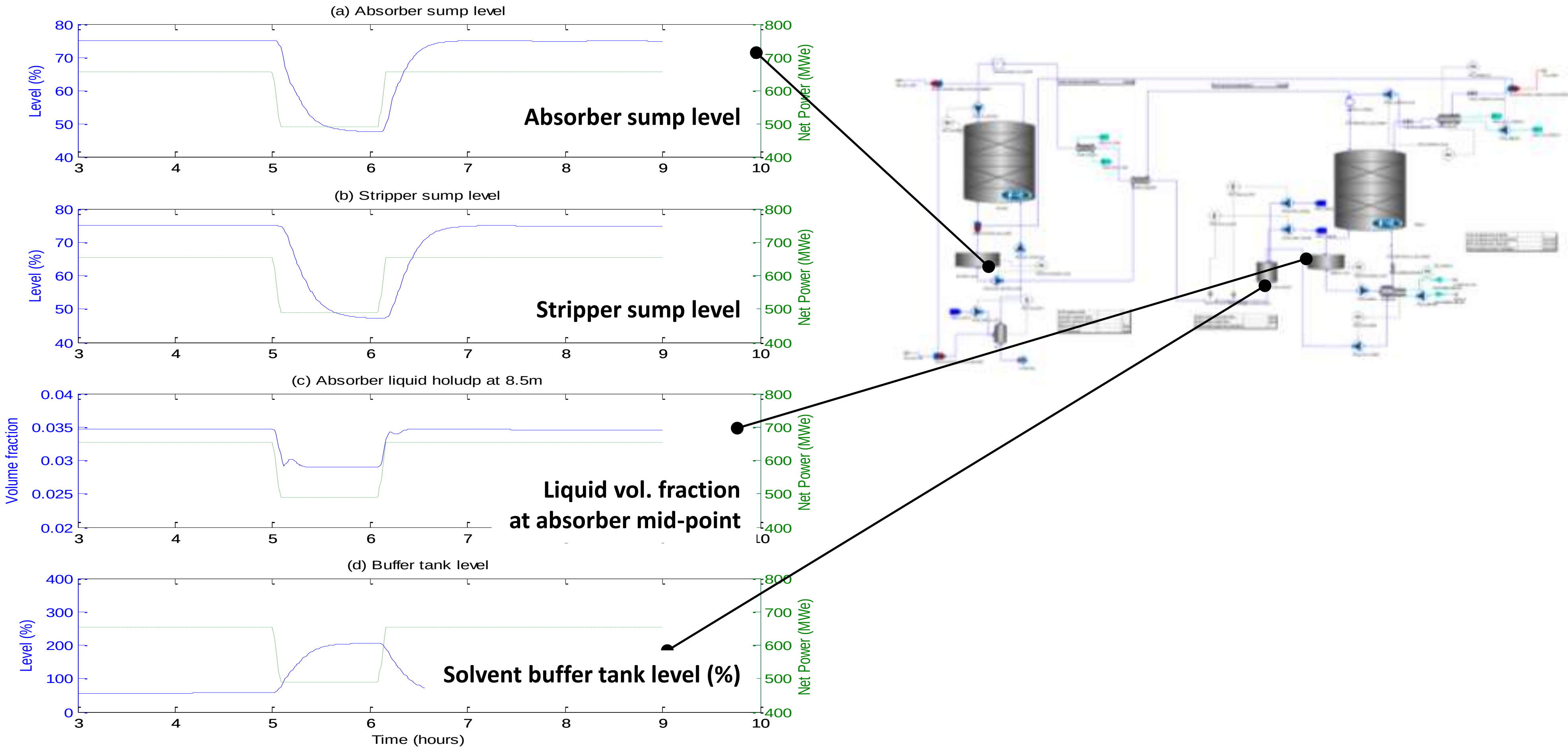


Dynamic analysis

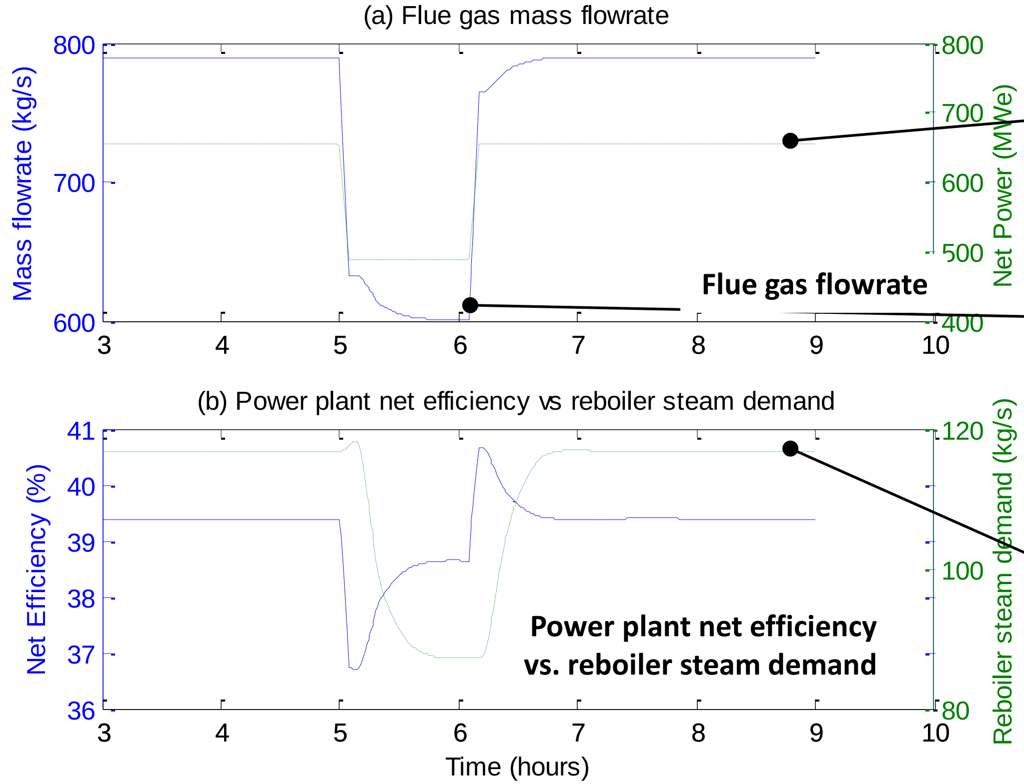
CO_2 capture plant

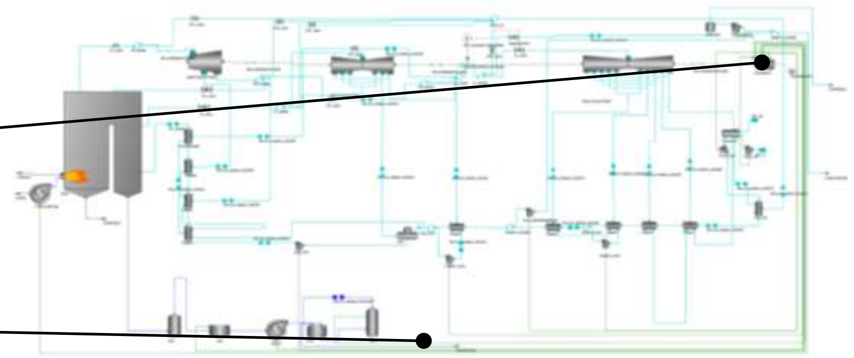


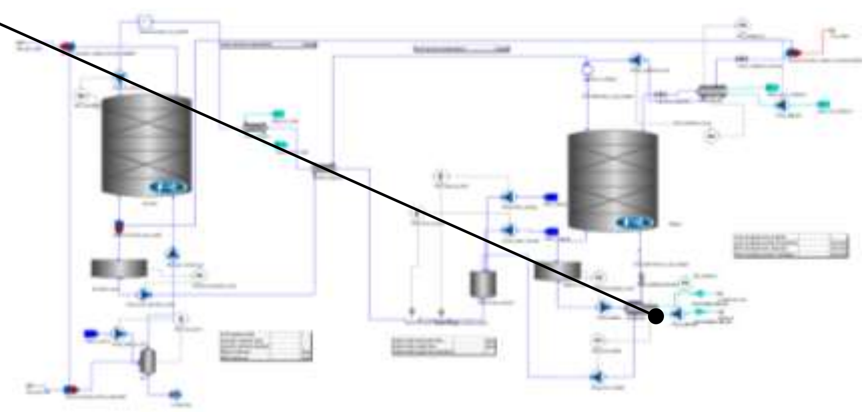
CO_2 capture plant



Power/CO_2 capture two-way coupling

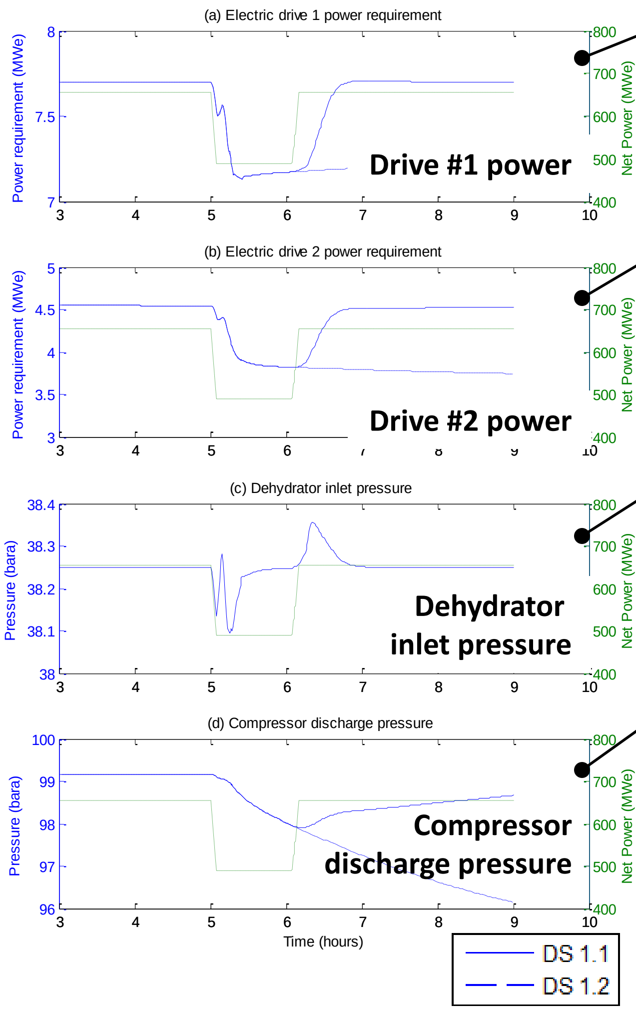


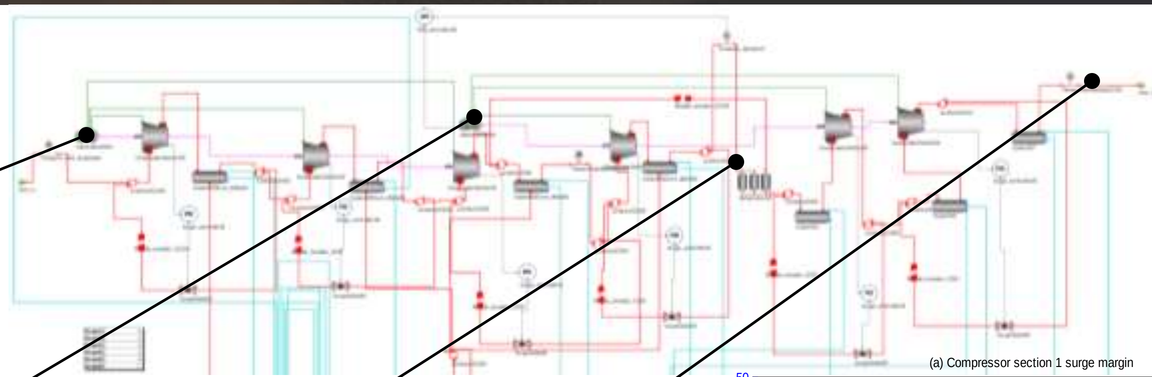


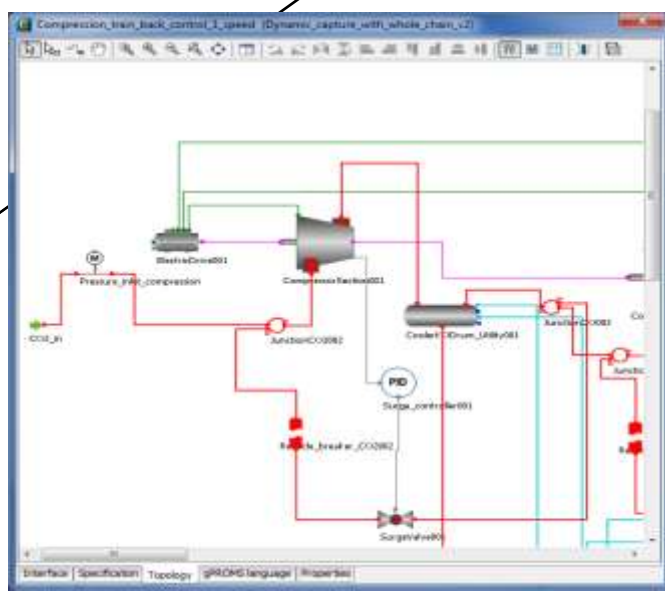


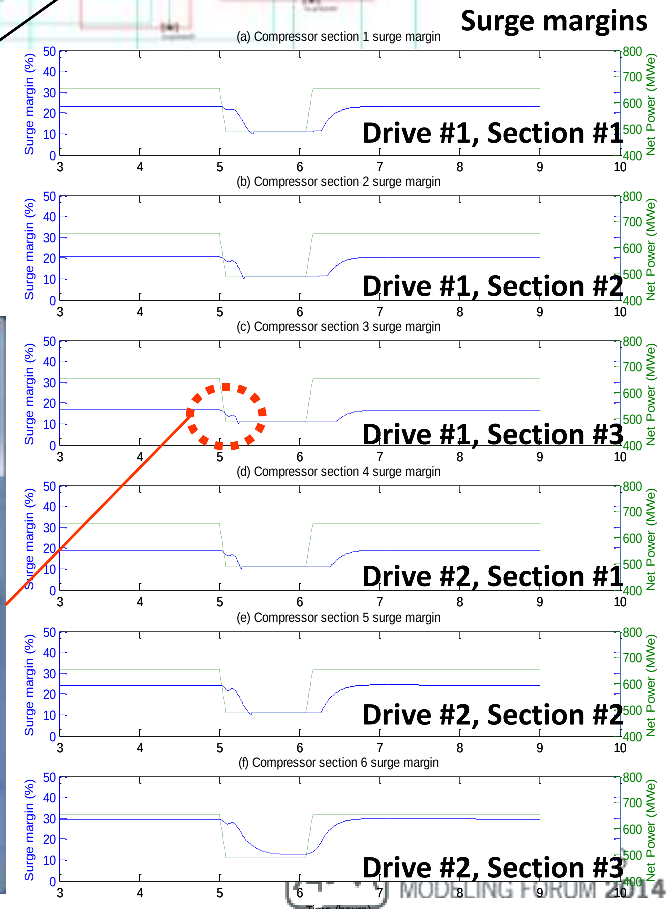
Dynamic analysis

CO_2 compression plant



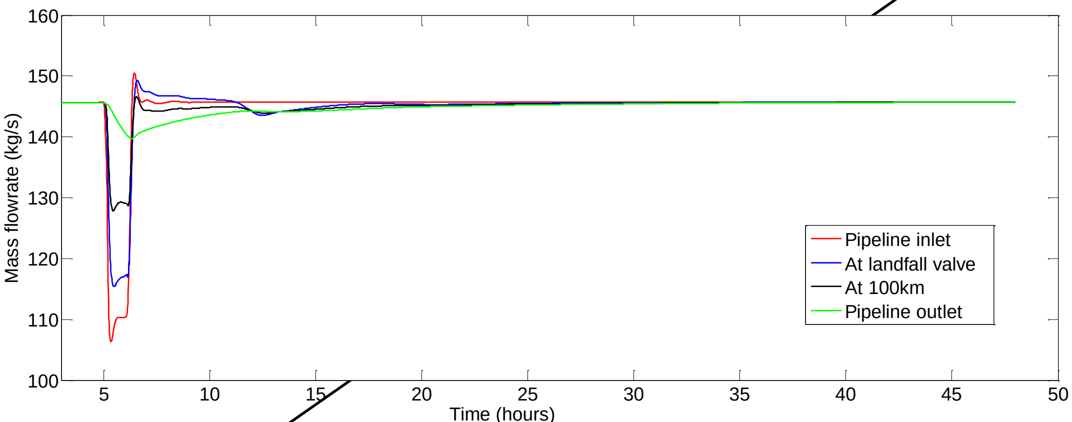


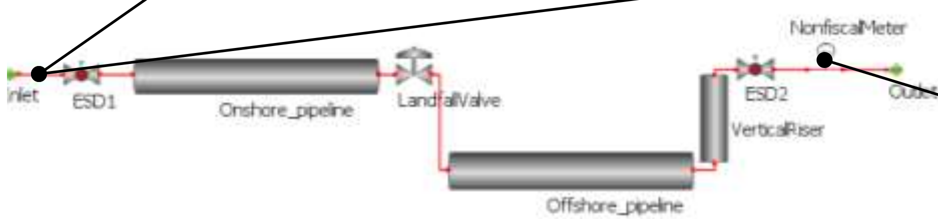


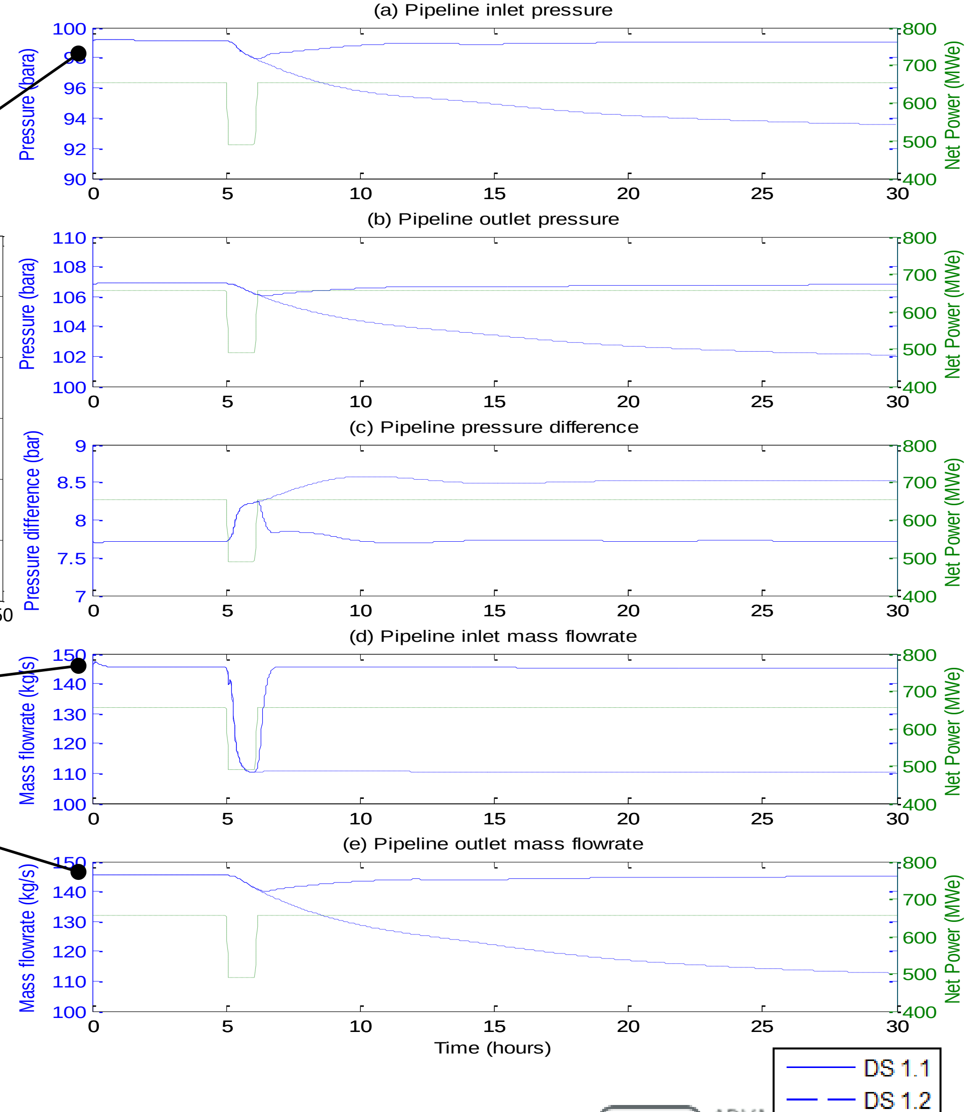


CO_2 transmission pipelines

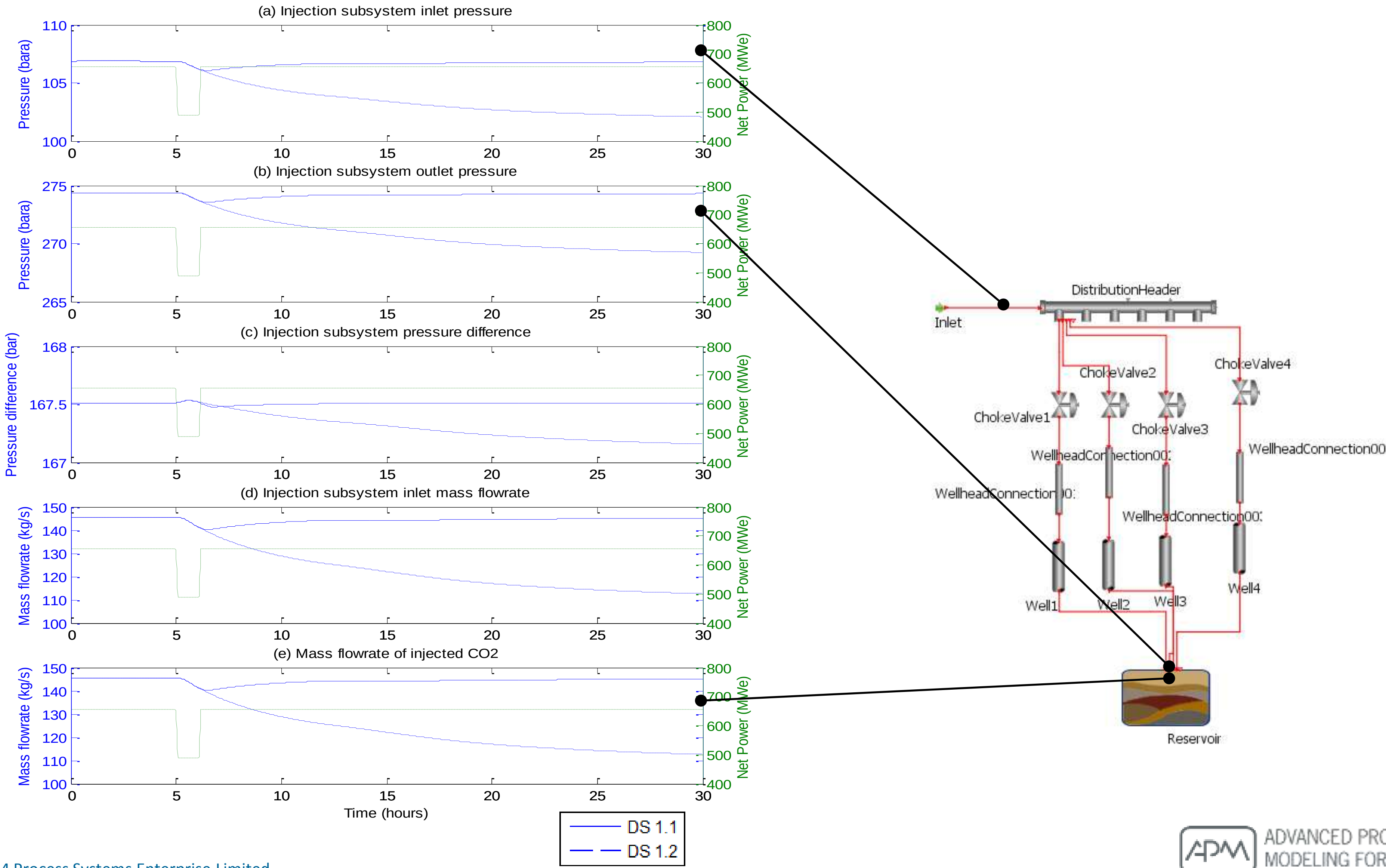
- Buffer potential for flexible operation







Dynamic analysis
CO_2 injection & storage



ADVANCED PROCESS MODELING FORUM 2014

Case Study: CCS network

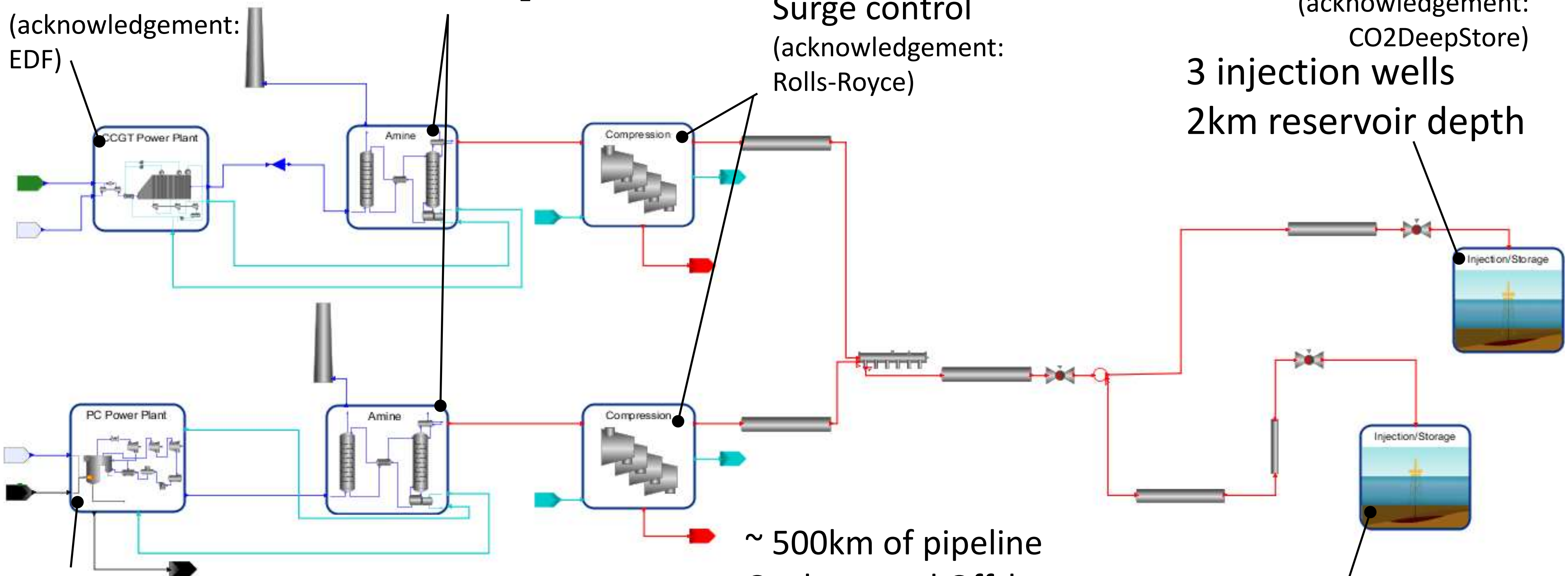
System overview

~740MWe
Combined Cycle
Gas Turbine
(acknowledgement: EDF)

Chemical absorption
MEA solvent
90% CO_2 capture

4 and 2 compression trains
2 frames per train
Surge control
(acknowledgement: Rolls-Royce)

Offshore dense-phase injection
(acknowledgement: CO2DeepStore)
3 injection wells
2km reservoir depth

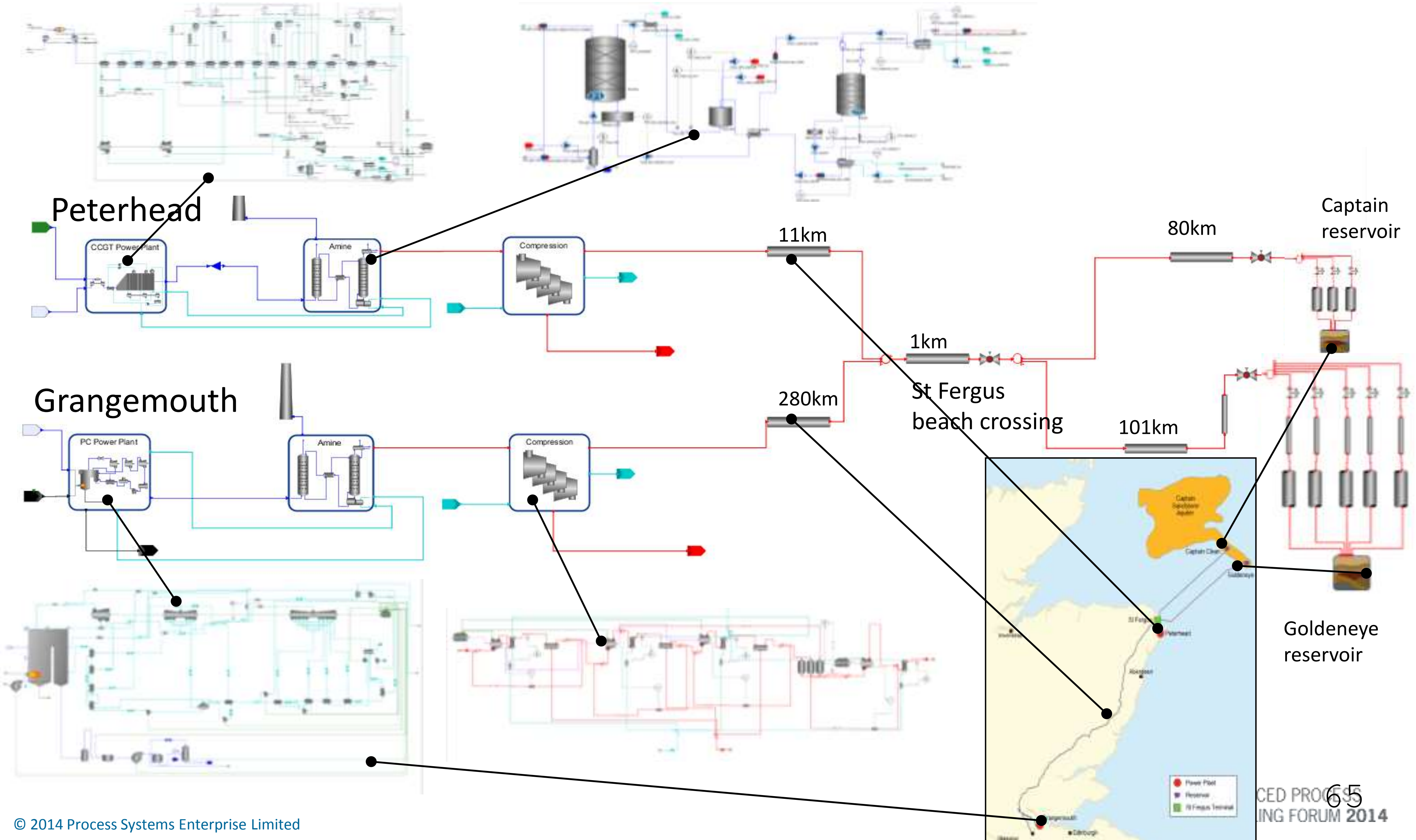


~ 500km of pipeline
Onshore and Offshore

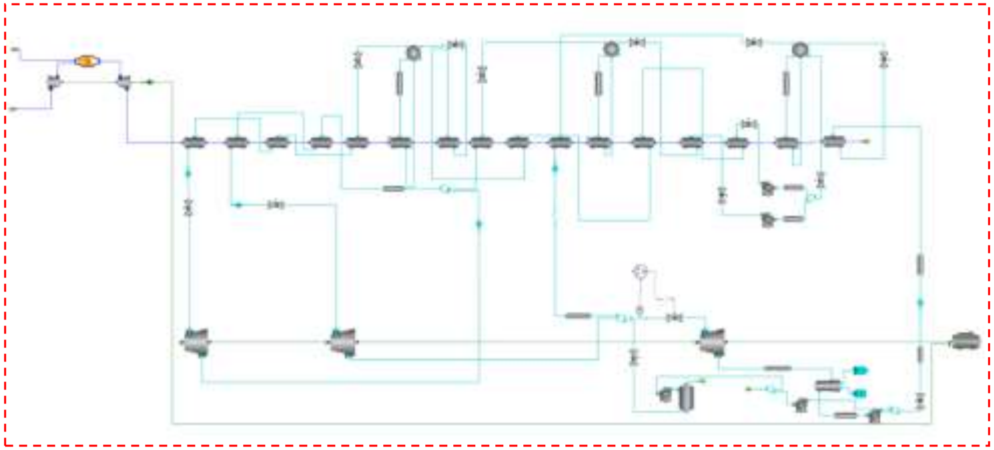
~800MWe
Supercritical
Pulverized coal
(acknowledgement: E.ON)

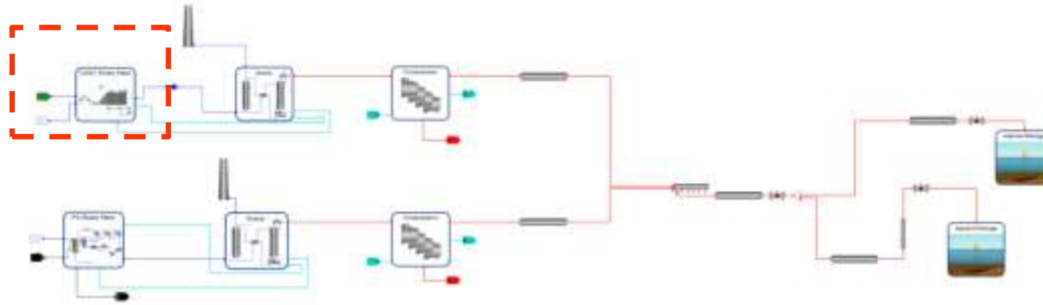
5 injection wells
2.6km reservoir depth

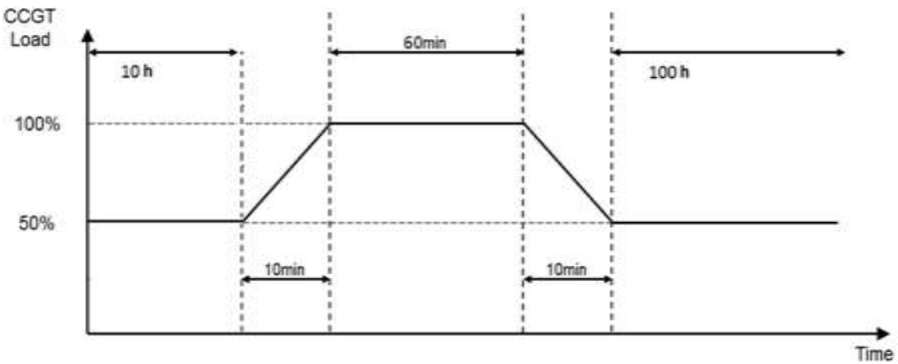
CCS network configuration

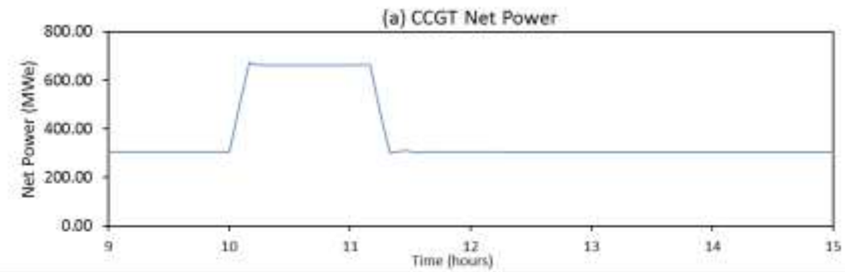


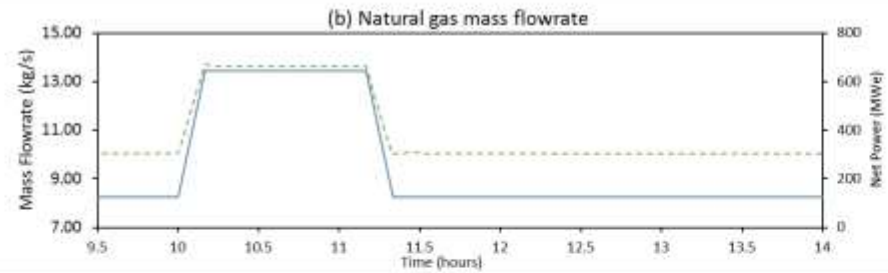
Load disturbance in CCGT

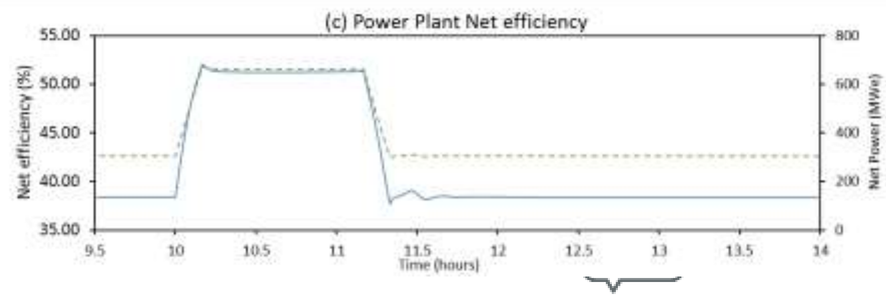




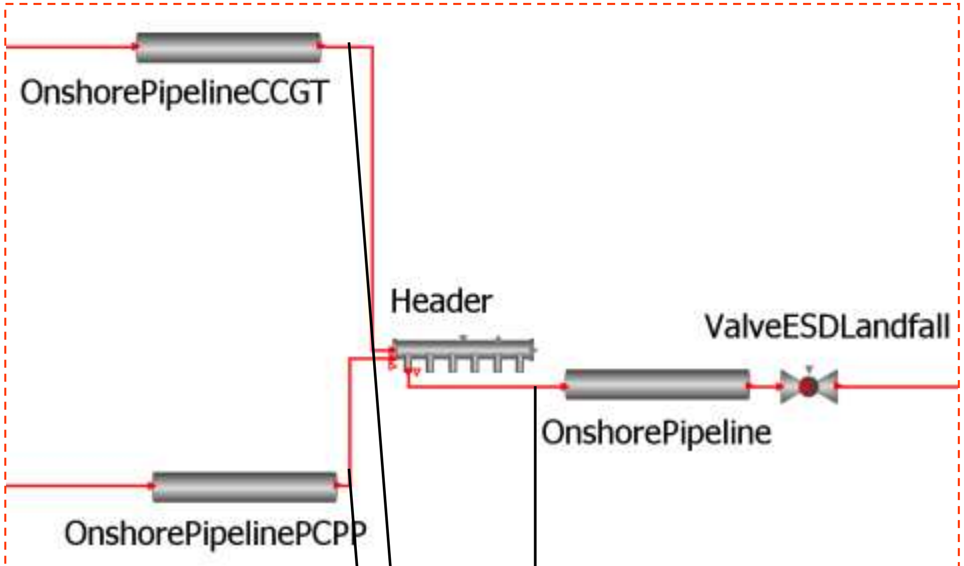


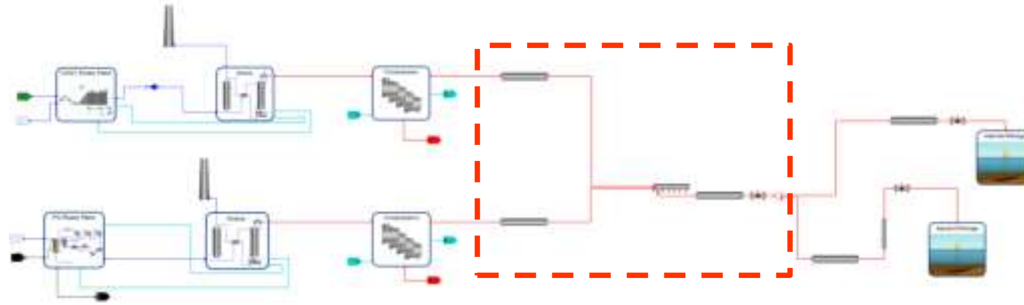




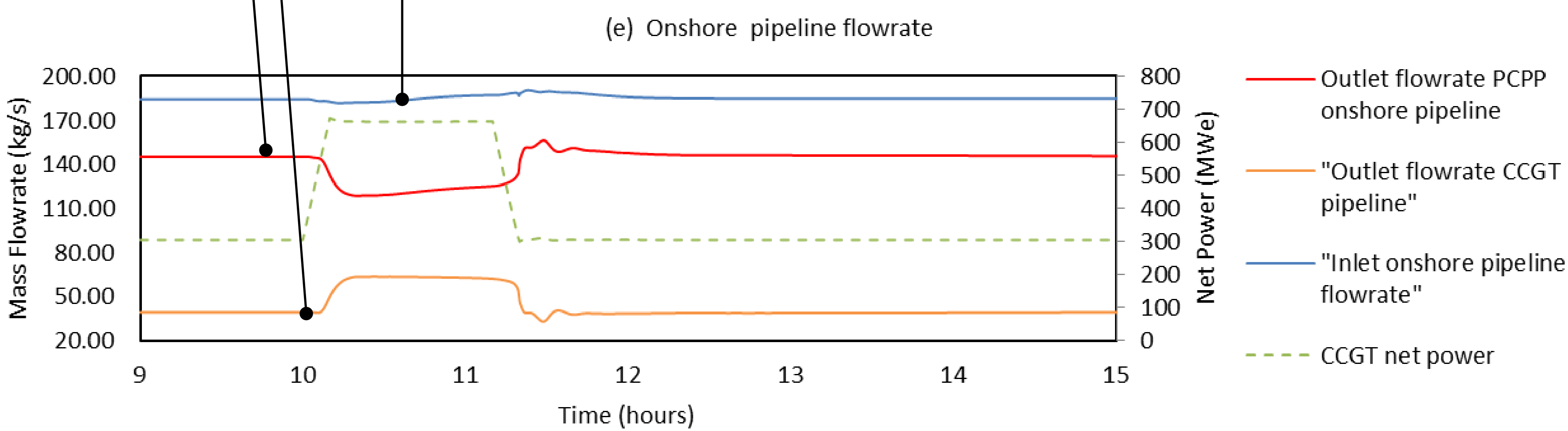


Load change effects





An increase of about 62% in the CCGT onshore pipe flowrate only increases 1.8% the inlet flowrate of the onshore pipe



Conclusions

Conclusions

- **Model-based engineering of CCS systems**
  - diverse stakeholders with different concerns & priorities

  ➔ need for coordination
- **System modelling is an essential tool**
  - inform and aid the design of safe control systems and operating procedures
  - identify areas requiring additional attention when designing for dynamic operation

- **An integrated modelling tool**
  - Capture, formalise & deploy existing knowledge on CCS technology
  - Common language for communication
  - Open architecture➔ allow incorporation of future technology

Conclusions

elementenergy

CARBON COUNTS

PSE

Imperial College London

The University Of Sheffield.

Demonstrating CO_2 capture in the UK cement, chemicals, iron and steel and oil refining sectors by 2025: A Techno-economic Study

Final report

for

Carbon Capture Journal

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gCCS system modelling technology used for Shell Peterhead project

Aug 10 2014

Shell Peterhead CCS project will be the first commercial UK user of PSE's gCCS systems modelling environment for whole-chain CCS design and operation.

gCCS is the world's first process modelling environment for support of design and operating decisions across the full CCS chain, from power generation through CO2 capture, compression and transport to injection. It is specifically designed to allow developers across the chain to address issues of interaction and interoperability between different chain components.

The gCCS software will be used during the Front-End Engineering Design (FEED) study phase of Shell's Peterhead CCS demonstration project to provide insight into the transient behaviour of the amine-based capture unit, and its effect on operations when integrated within the full system. In particular it will help to demonstrate the flexibility of the capture process design within the wider CCS chain through simulation of normal and off-design operational scenarios, and thus help reduce technology risks in this first-of-a-kind CCS project.

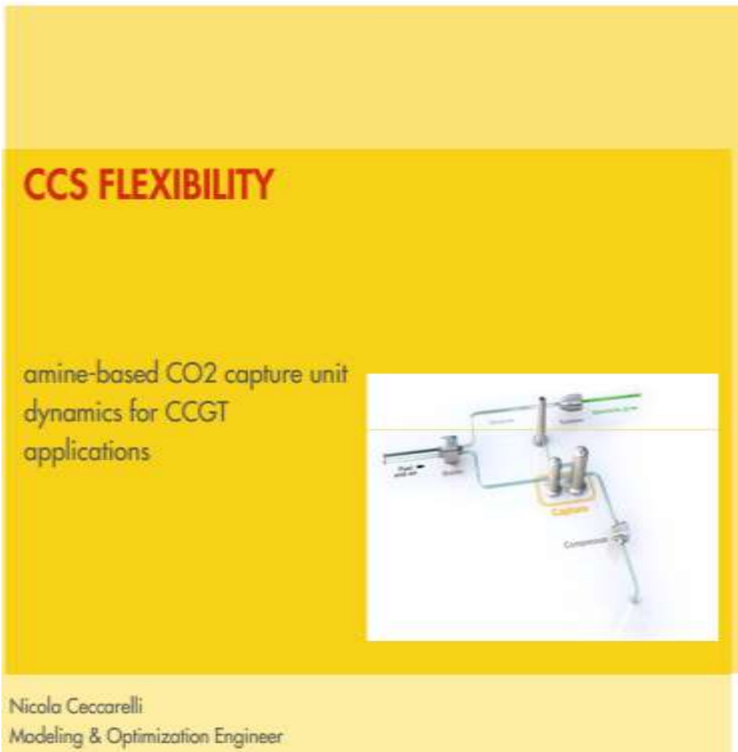
Alfredo Ramos, PSE's head of Power & CCS and leader of the development, said, "this is precisely the type of large-scale CCS application that gCCS was developed to support. For the first UK commercial use, we are very pleased to see it being used on such an important development."

gCCS is the commercially-supported product resulting from the £3m Energy Technologies Institute (ETI) funded CCS Systems Modelling Tool-kit project. The project was established to support the future design, operation and roll-out of cost-effective CCS systems in the UK and involved E.ON, EDF, Rolls-Royce, CO2DeepStore, PSE and E4tech.

Process Systems Modelling

Conclusions

- Shell - CCS flexibility
  - Full start-up and shutdown studies



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GHGT-12

Flexibility of low-CO_2 gas power plants: Integration of the CO_2 capture unit with CCGT operation

Nicola Ceccarelli, Monica van Leeuwen, Tanja Wolf, Peter van Leeuwen, Rick van der Vaart, Wilfried Maas[a], Alfredo Ramos[b]

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Acknowledgements

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  - Energy Technologies Institute
  - E.On
  - EDF
  - Rolls-Royce
  - CO2DeepStore
  - E4Tech

Thank you