

Evaluation and Demonstration of Commercialization Potential of Carbon Capture Simulation Initiative Tools within gPROMS Advanced Simulation Platform

Alfredo Ramos, Vice President Energy & Environment



- Carbon Capture Simulation Initiative
- CCSI Commercialization Project (FE0026307)
- Role of advanced process/systems modelling
- PSE background – why us?
- Project status update
- Summary

Advanced Process Modelling initiatives aimed at CCS

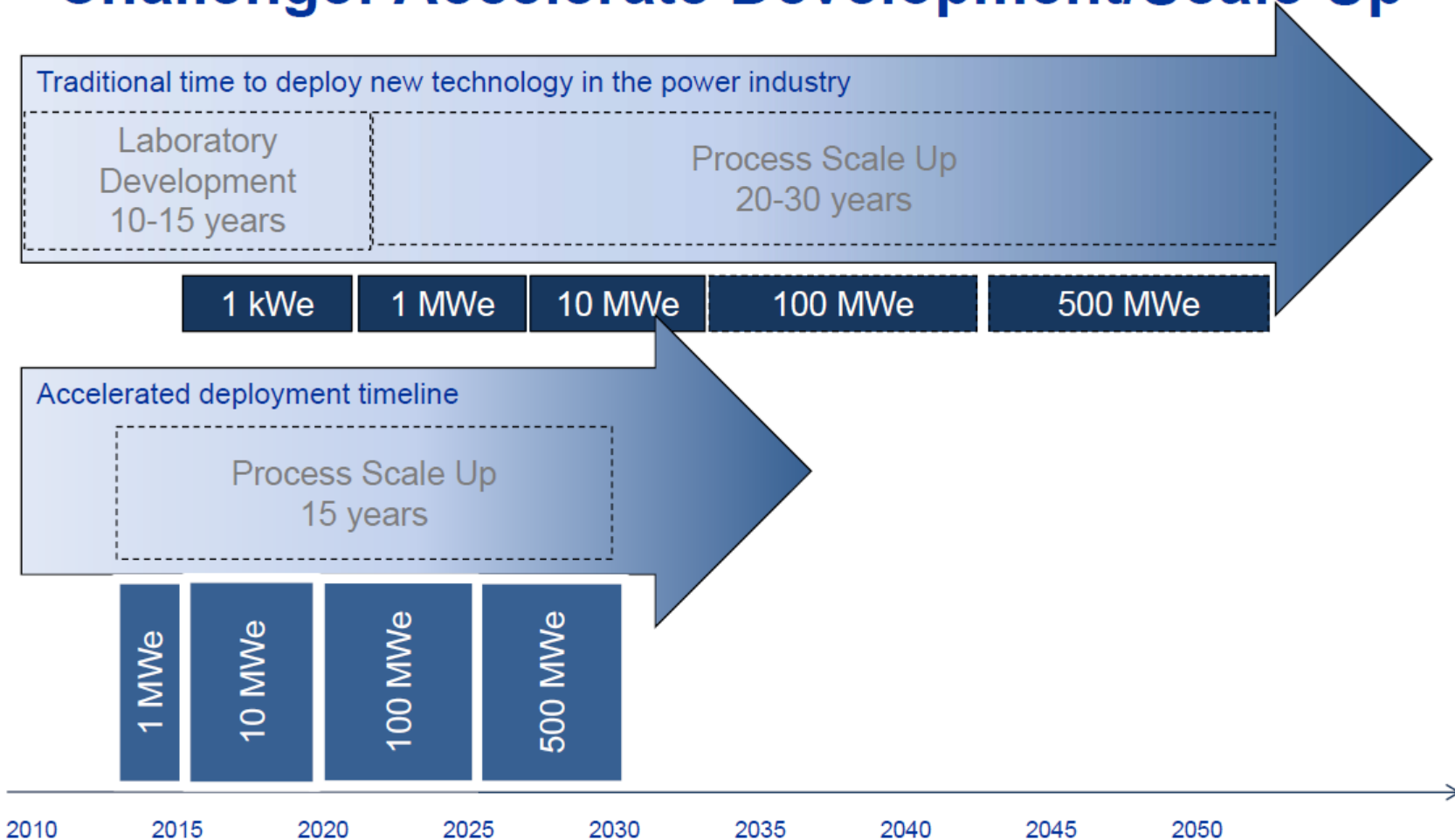
2. Carbon Capture Simulation Initiative (CCSI)



U.S. Carbon Capture Simulation Initiative (CCSI)



Challenge: Accelerate Development/Scale Up



U.S. DEPARTMENT OF ENERGY

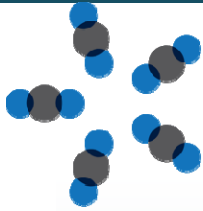
Goals & Objectives of CCSI



- **Develop** new computational tools and models to enable industry to more rapidly develop and deploy new advanced energy technologies
 - Base development on industry needs/constraints
- **Demonstrate** the capabilities of the CCSI Toolset on non-proprietary case studies
 - Examples of how new capabilities improve ability to develop capture technology
- **Deploy** the CCSI Toolset to industry
 - Initial licensees, CRADA

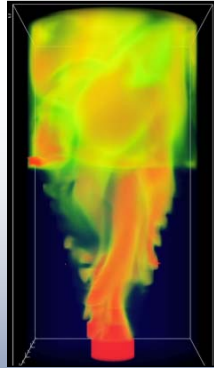
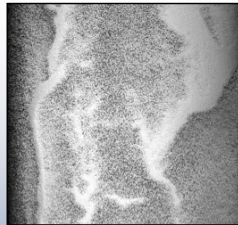
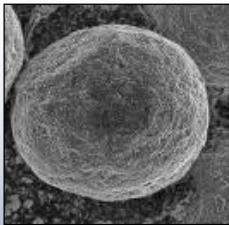


U.S. Carbon Capture Simulation Initiative (CCSI)



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



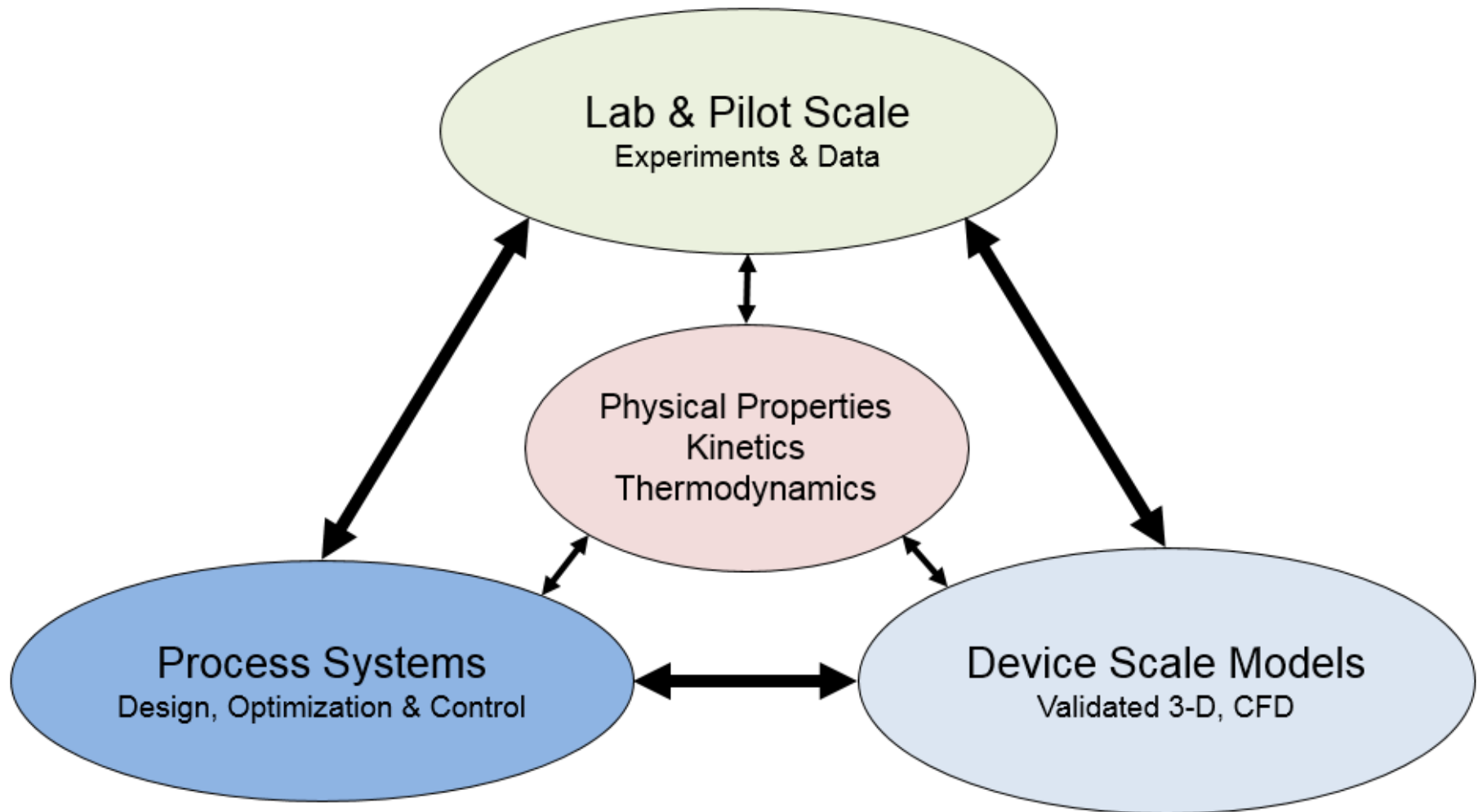
Academia



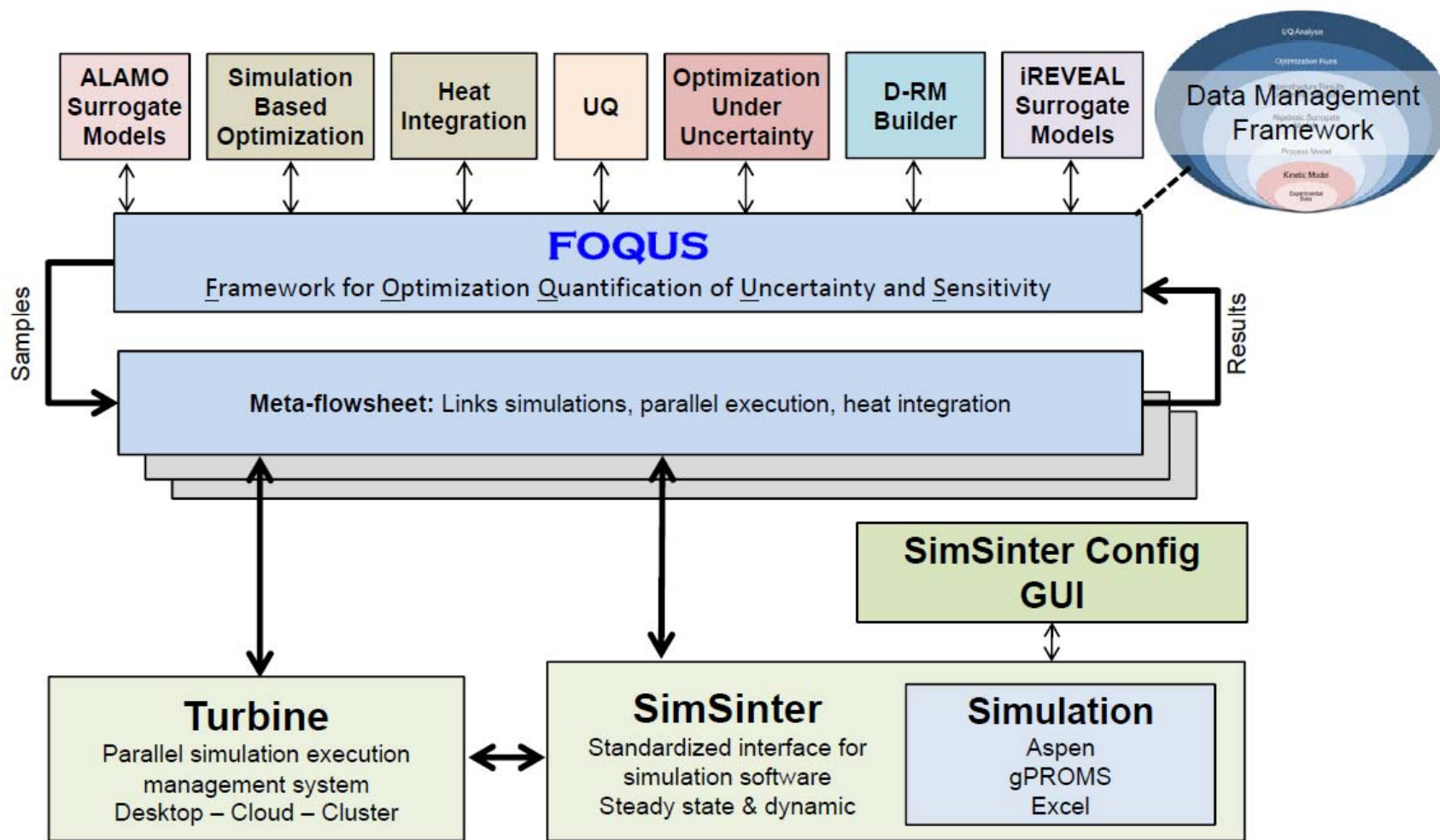
Industry



Advanced Computational Tools to Accelerate Carbon Capture Technology Development



U.S. Carbon Capture Simulation Initiative (CCSI) Framework & technologies



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. Sirola and G. P. Towler Elsevier.



U.S. DEPARTMENT OF ENERGY

CCSI Toolset Commercialization Project – DoE

Award Number FE0026307



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- 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

- Expand Power & CCS offering
 - Enhancements to gCCS and gPOWER products
 - Supporting Advanced Energy Systems initiatives (Fuel Cells)

- Deploy CCSI tools and models beyond CCS applications
 - Chemicals and petrochemicals (energy management)
 - Life sciences
 - Oil & Gas

Project team/stakeholders



Project partners ...and team



Alejandro Cano, PhD
Principal Investigator
Technical focal point

Alfredo Ramos, MBA, MSc
Co-Principal Investigator
Commercialization



Ade Lawal, PhD
Project Manager
Coordinator Process Modelling task

Pieter Schmal, PhD
Principal Applications Engineer
Coordinator ALAMO/FOQUS



Debangsu Bhattacharyya, PhD
Co-Principal
Task leader Process Modelling

David Mebane, PhD
Co-Principal
Task leader Sorbentfit/SolventFit



Prof Nick Sahinidis
Co-Principal
Task leader ALAMO

Key external stakeholders



■ Organisations



■ People

- Jason C. Hissam (NETL Project Officer)
- Ashley Reichl (U.S. Contract Specialist)
- David Miller as initial (introductory) point of contact for non-fast track tools

Key external stakeholders



- Industry advisory board members



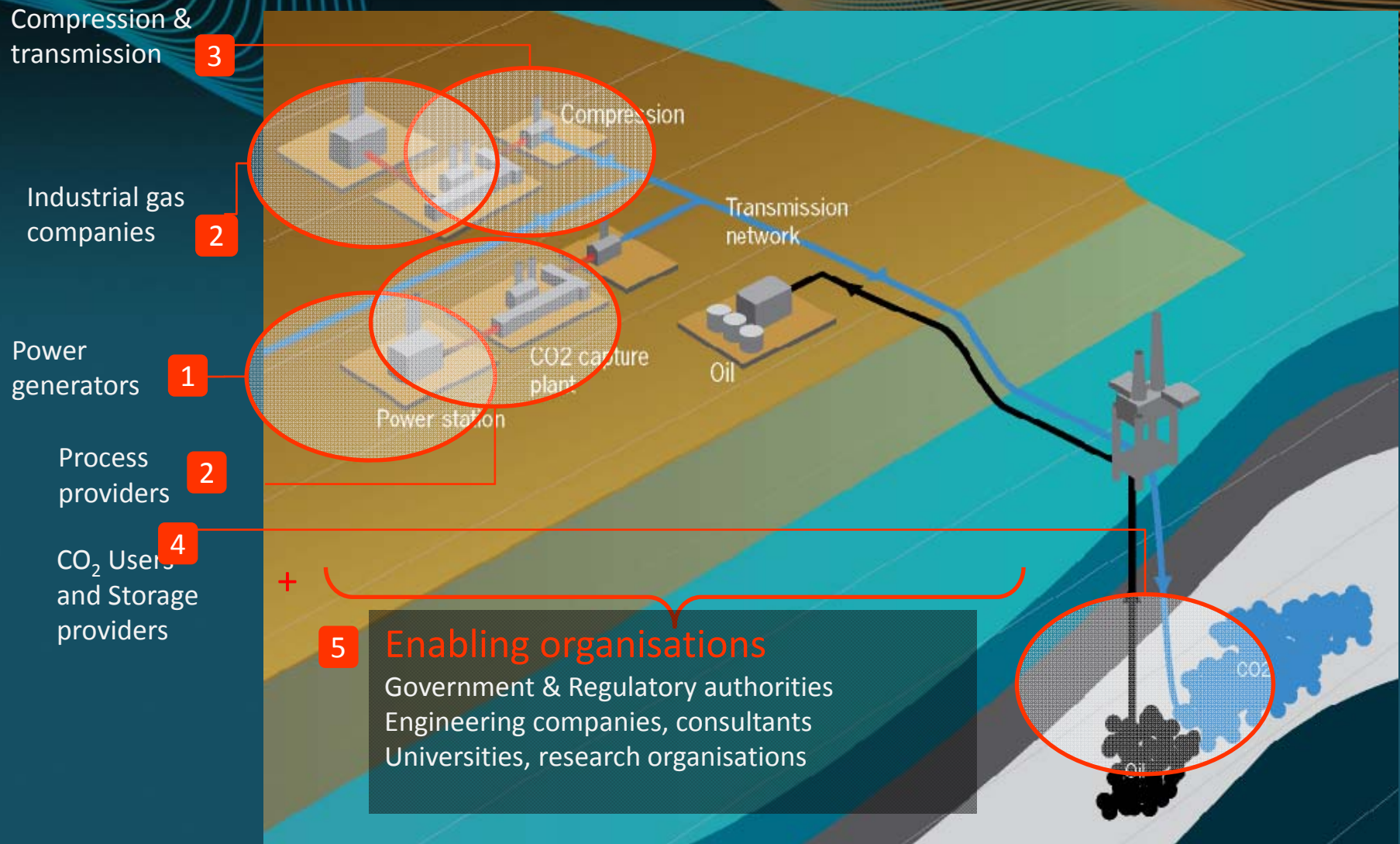
- Uncertainty quantification approach essential in guiding R&D efforts to minimise cost of low-emission energy systems
 - Focus on what really matters

- Seamless integration of data-driven and first-principles models streamlines lifecycle of models/modelling tools
 - Extend range of application of model-based solutions
 - Accelerate deployment of innovative, low-carbon energy systems
 - Optimal design and operation of CCS and other advanced energy systems, reducing transition cost to low-carbon economy

Challenges to the roll-out of Carbon Capture Utilization and Storage (CCUS)



CCSU challenges – stakeholders



CCS challenges

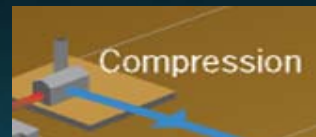
Multiple stakeholders with different issues & challenges



- Grid demand
- Flexibility
- Efficiency
- Fuel mix
- Trip scenarios



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



- Optimal operating point
- Efficiency
- New design
- Impurities
- Control
- Safety

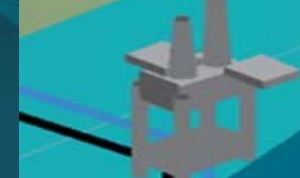


- Composition effects
- Phase behavior
- Capacity
- Buffering / packing
- Routing
- Safety
- Depressurisation
- Control
- Leak detection

Government

- Policy
- Strategic
- Infrastructure development
- H&S

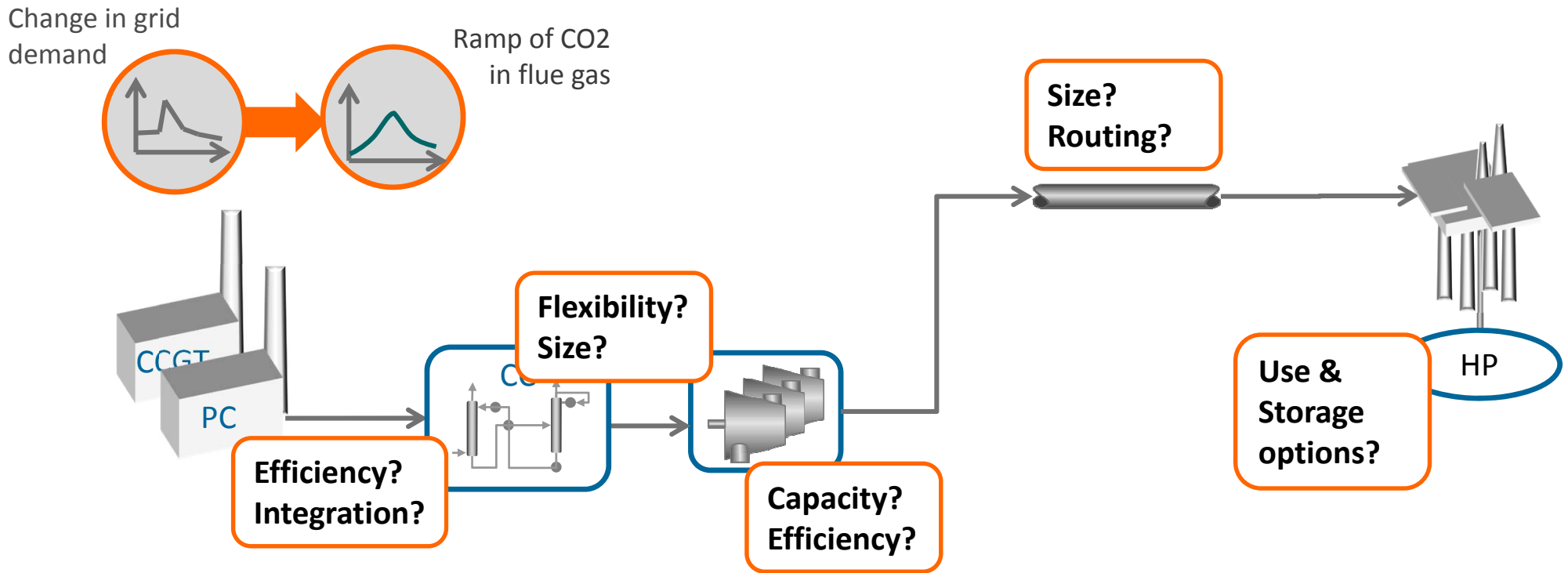
Injection/storage



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

...currently being addressed by individual tools

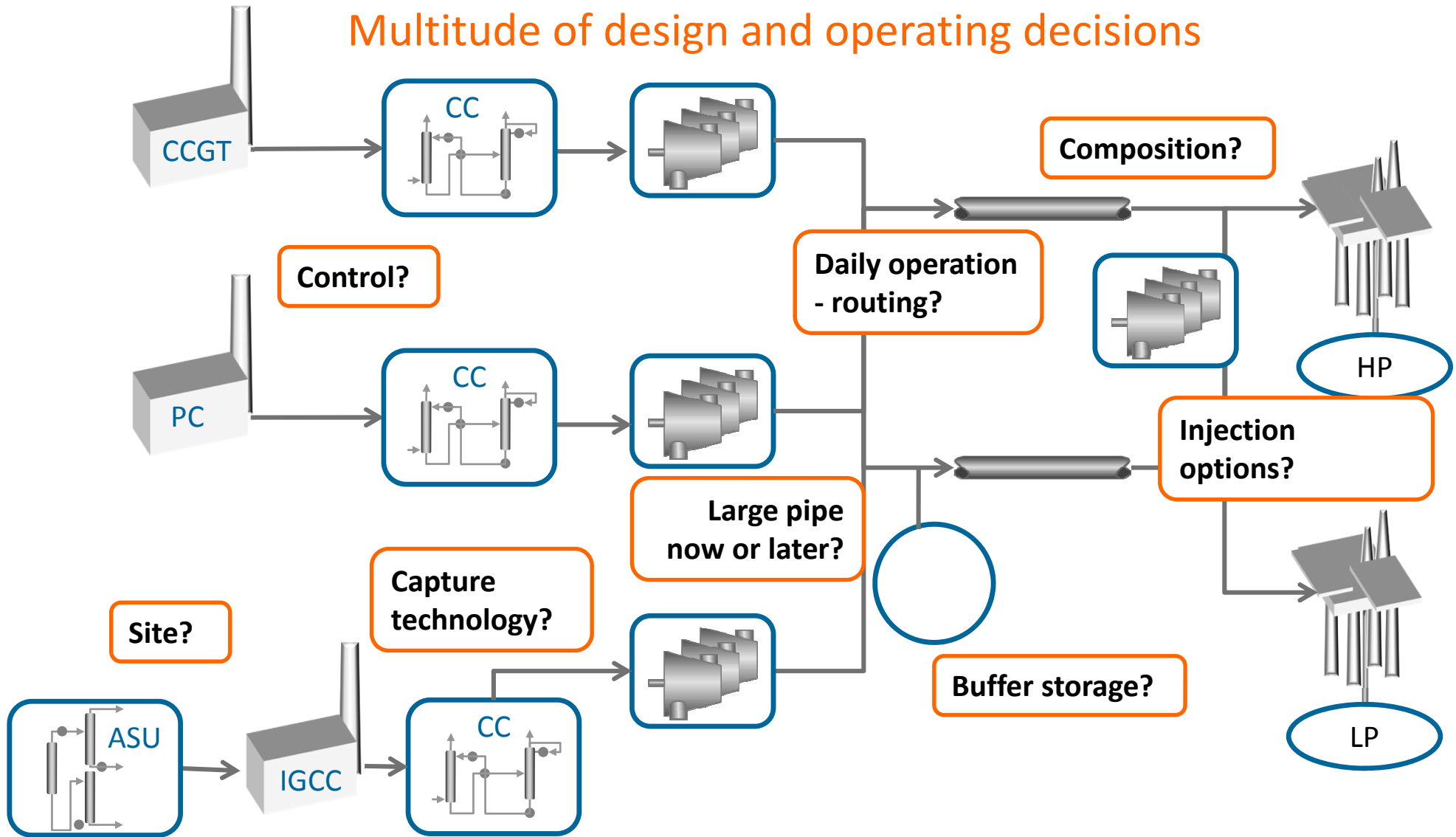
Challenges – ‘interconnectedness’ (I)



Now all connected CO2 network as well

Challenges – ‘interconnectedness’ (II)

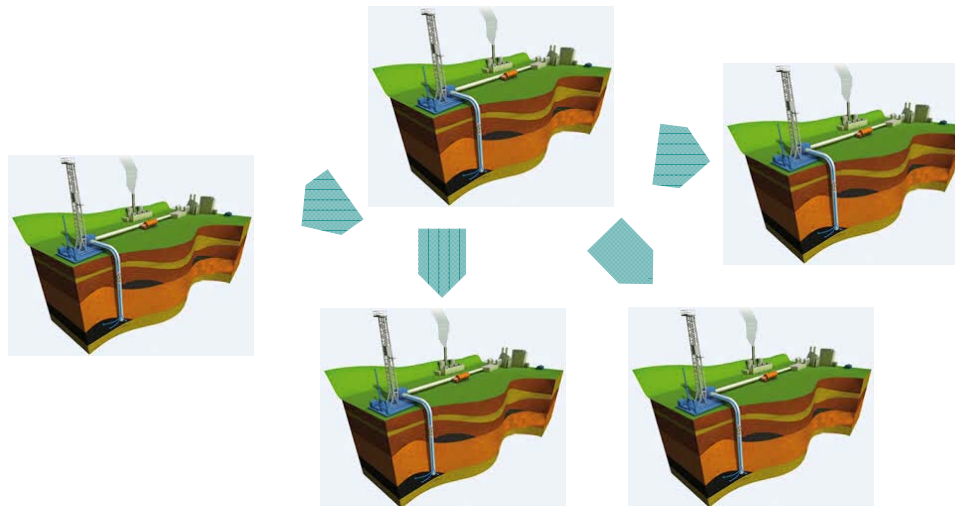
Multitude of design and operating decisions



Challenges – ‘transferability of experience/expertise’ (I)



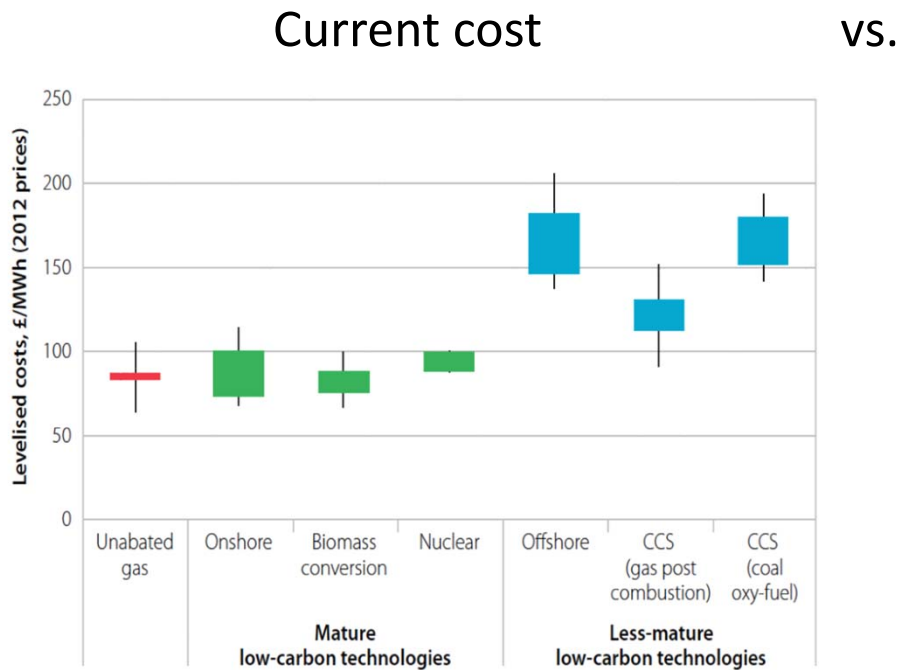
- Substantial challenges in moving from first-of-a-kind (FOAK) to Nth-of-a-kind (NOAK) owing to “uniqueness” of each CCS project
 - CO₂ sources
 - Topography / pipeline layout
 - CO₂ store’s geological characteristics
- Advanced process modelling is essential to translate experience from one large-scale integrated project to the next



Challenges for CCS – ‘cost’ (I)



- Current cost of abatement of CCS too high with respect to other low-carbon technologies/ renewables
- ...particularly when put in perspective with electricity price

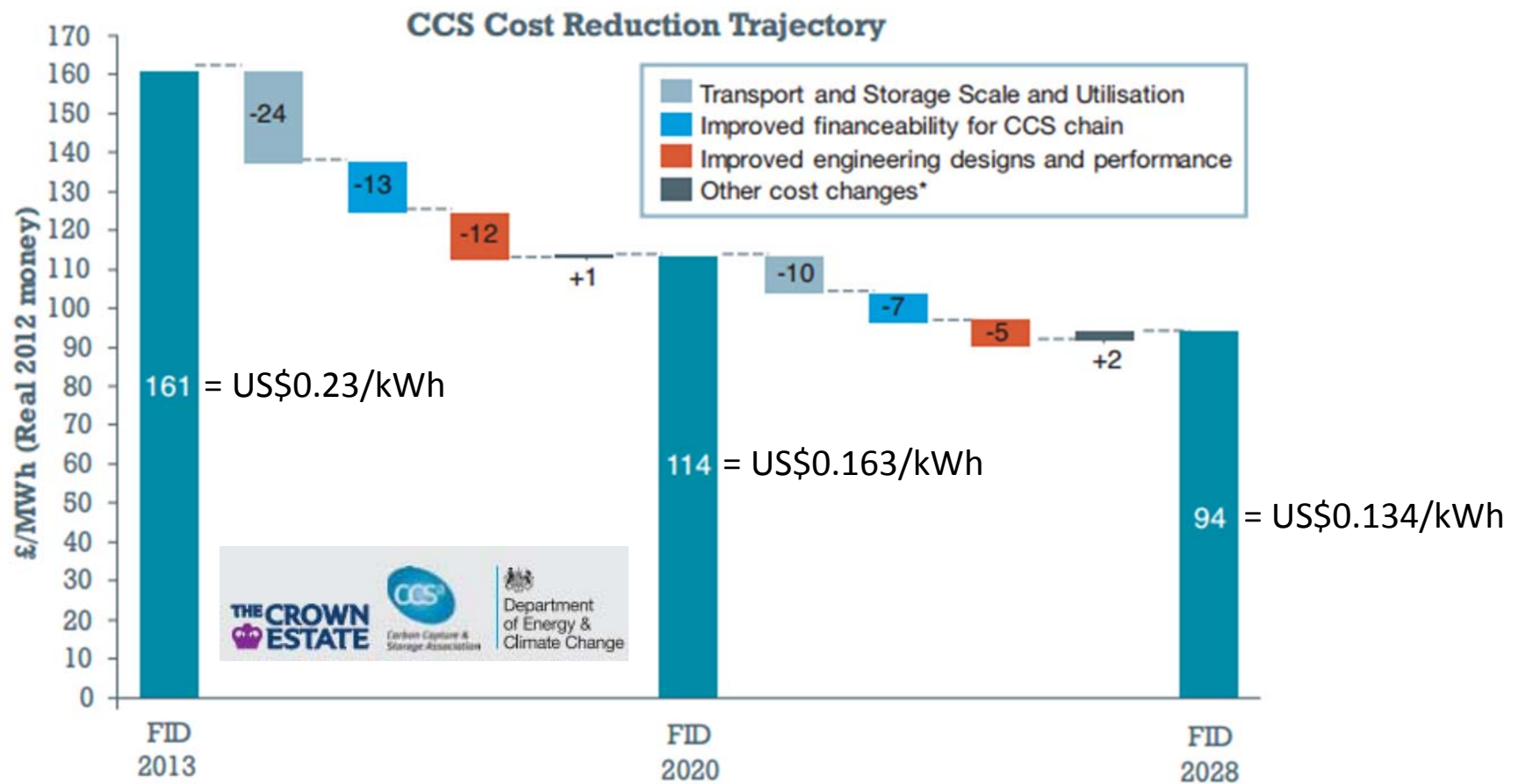


Challenges for CCS – ‘cost’ (II)



■ Outlook 2030 – there is hope!

- UK’s CCS Cost Reduction Taskforce identified potential for US\$0.024/kWh* directly attributable to improved engineering designs and performance



Source: UK Cost Reduction Taskforce Final Report – May 2013

* Exchange rate: USD/GBP = 0.7

Putting these all together ...



System-wide modelling is a key technology for addressing these questions and investigating **whole-chain** or **partial-chain interaction**

... by providing **accurate quantification** for **decision support**

PSE BACKGROUND: FROM RESEARCH TO INDUSTRY

1997



Company 'spins out' off Imperial College
Private, independent company
incorporated in UK



Acquires technology

2007



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

2015



International company delivering software and services
Major process industry focus
Strong R&D

Established sectors



Chemicals & Petrochemicals



Oil & Gas



Formulated Products



Energy & Environment

Strategic initiatives



Americas

Air Products
Air Liquide
BP Chemicals
Carus Corporation
CB&I
ConocoPhillips
DuPont
ExxonMobil
Ineos
Infineum
KBR
Praxair

Argonne National Lab
Ballard
Boehringer Ingelheim
Eli Lilly
Energy Solutions
Folgers
Genentech
Johns Manville
Marck
Millennium
Mylan
Pfizer
Sandoz
Santitas
Santitas
Santitas

ExxonMobil
PRAXAIR
ConocoPhillips
DUPONT
P&G
Lilly
Pizer
Santitas

EMEA

AMEC
Ariaema
AstraZeneca
BP Chemicals
BP Exploration
CEPSA
Chiriant
Deed Sea Works
E.ON
EDF
Johnson Matthey
Meerck
PDO
Perenco
Petrofac
Repsol
SABIC
SASOL
Shell
Siemens VAI
Solvay
SINTEF
Subzer
TOTAL

AngloAmerican
ARKEMA
BASF
AWE
Infineum
SABIC
REPSOL
SIEMENS
Shell
TOTAL
AstraZeneca
gsk
Nestle

APAC

MITSUBISHI CHEMICAL
GS E&C
Hamwha Chemical
Hyosung
Hyundai HI
JGC
KIOST
KRIOK
LG Chem
Lotte Chemical
Mitsubishi Chemical
Posco Energy
RIST
Samnam Petrochemical
Samsung BP
SCG
SK Chemicals
SK Innovation
SK Petrochemicals
Sungul China
Taiyo Nippon Sanso

LG Chem
HYUNDAI
JGC
TAIYO NIPPON SAN SO
SAMSUNG
HONDA
TOYOTA
DENSO

Allinchem
DSP
Dongas
Honda
KIOK
Samsung Electronics
Samsung SDI
Toshiba Fuel Cell
Toyota CRDL
Toyota Motor Company

Sectors (verticals) and products



Oil & Gas



Chemicals & Petrochemicals



Formulated Products



Energy & Environment

General mathematical modelling

g|MODEL

gPROMS ModelBuilder
Advanced process modelling

g|FLARE

Flare networks & depressurisation

Oil major

g|PROCESS

gPROMS ProcessBuilder
Advanced process simulation

g|CRYSTAL g|SOLIDS g|COAS

Solids process optimisation

Crystallization process optimisation

Oral absorption modelling

Procter & Gamble

Pfizer

g|POWER g|FUELCELL g|CCS g|WATER

Power plant modelling

Fuel cell stack & system design

Carbon capture & storage

Water systems optimisation

Toyota

ETI

EPFL



THE WORLD'S LEADING ADVANCED PROCESS MODELLING PLATFORM



Molecular Systems Engineering
@Imperial College

High-fidelity modelling and optimisation tools for R&D, Engineering & Operations

Accelerate innovation • Optimise process design & operations • Improve R&D efficiency • Manage technology risk

Model-based Engineering

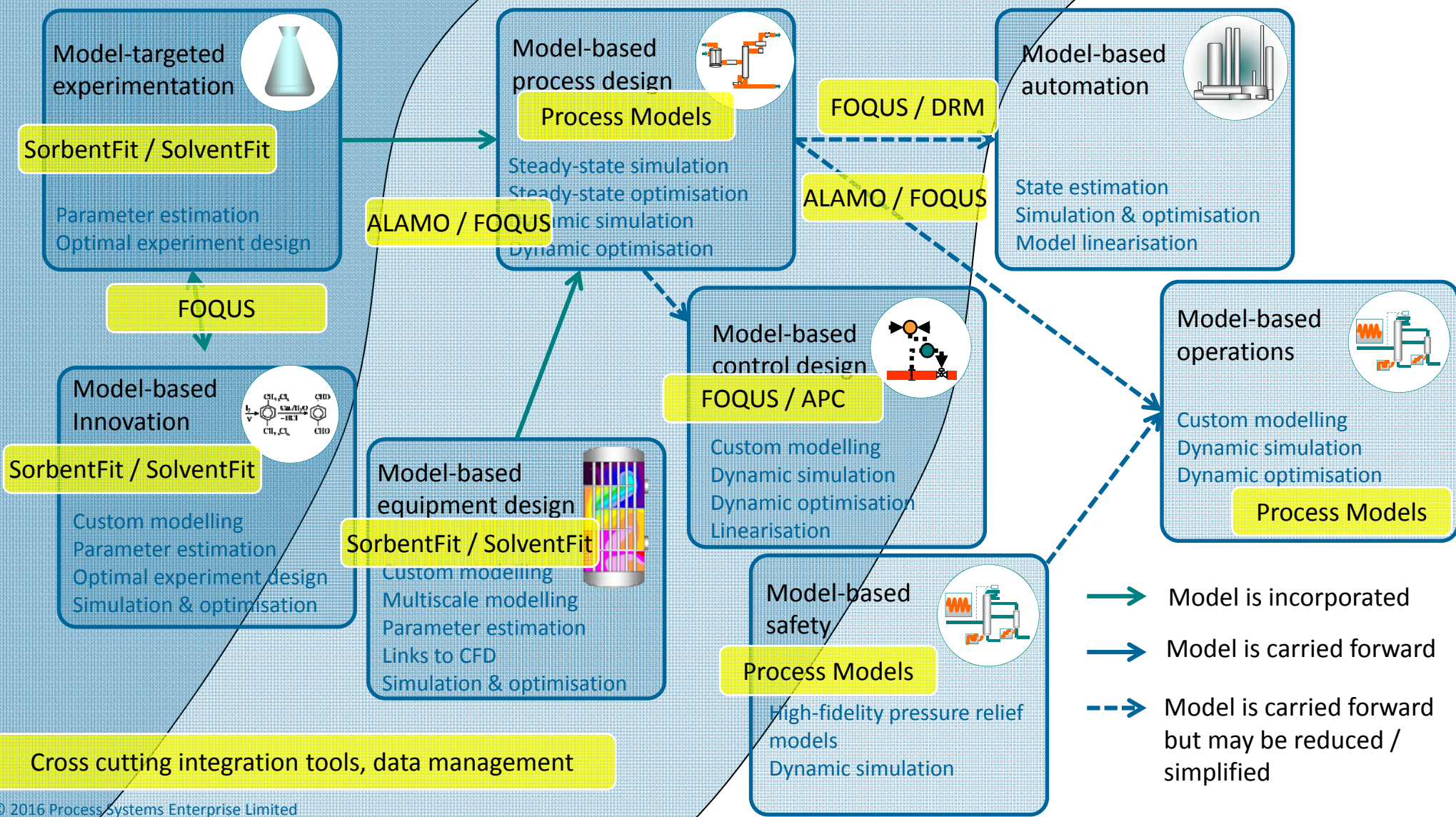
Technologies & workflows across the process lifecycle



Concept & discovery

Engineering design

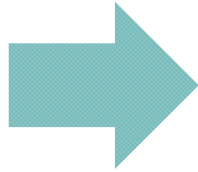
Operation



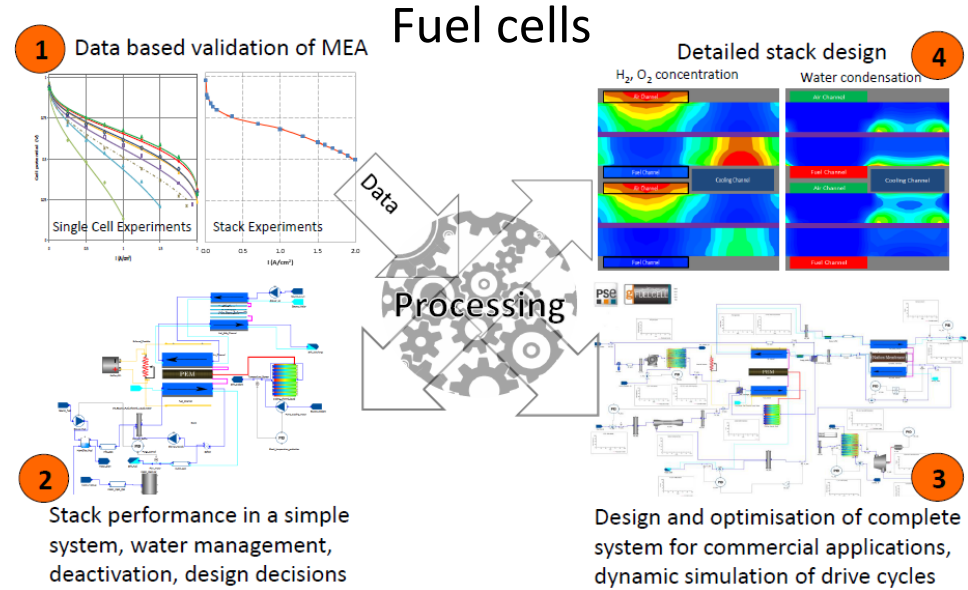
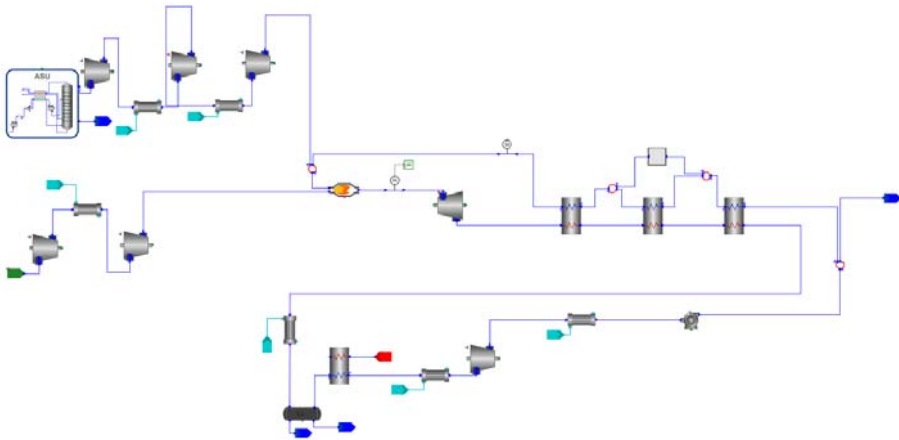
Applications



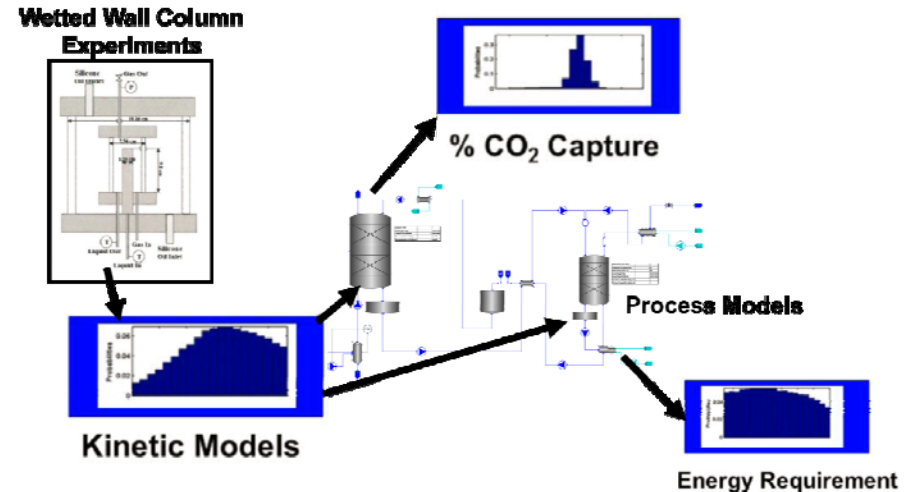
- Accelerate rate of cost reductions for low-emission technologies through deployment of models across the entire development lifecycle



Advanced Thermodynamic Cycles
(e.g. Allam)

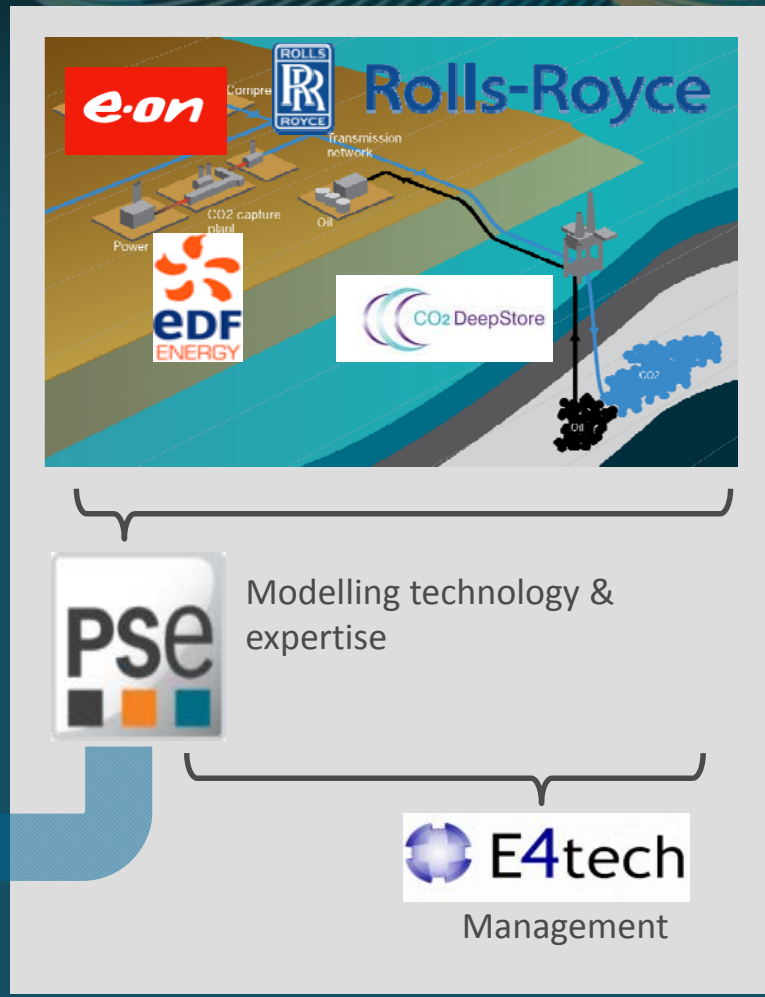


- Uncertainty Quantification extension of gCCS CO₂ Capture library (Morgan et al., 2015)



■ CCS Advanced Process Modelling Tool-kit Project

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



A screenshot of the PSE website homepage. The header includes the PSE logo, navigation links (Company, Concepts, Sectors, Products, Services, Contact), and the tagline "The power to be certain". The main content area features a photo of four men in suits, with the text "gCCS v1.0 released" and "World's first whole-chain CCS system modelling environment". Below this is a quote from the Secretary of State for Energy, Ed Davey. A "Find out more" button is visible. The footer contains a row of icons representing various sectors: Chemicals & Petrochemicals, Oil & Gas, Life Sciences, Power & CCS, Fuel Cells & Batteries, Food & Consumer, Specialty & Agrochemicals, Wastewater Treatment, and Academic.

■ Process models

- Power generation
 - Conventional: PC, NGCC
 - Non-conventional: oxy-fuelled, IGCC
- Solvent-based CO₂ capture
- CO₂ compression & liquefaction
- CO₂ transportation
- CO₂ injection in sub-sea storage
- CO₂ Enhanced Oil Recovery

■ Costing models

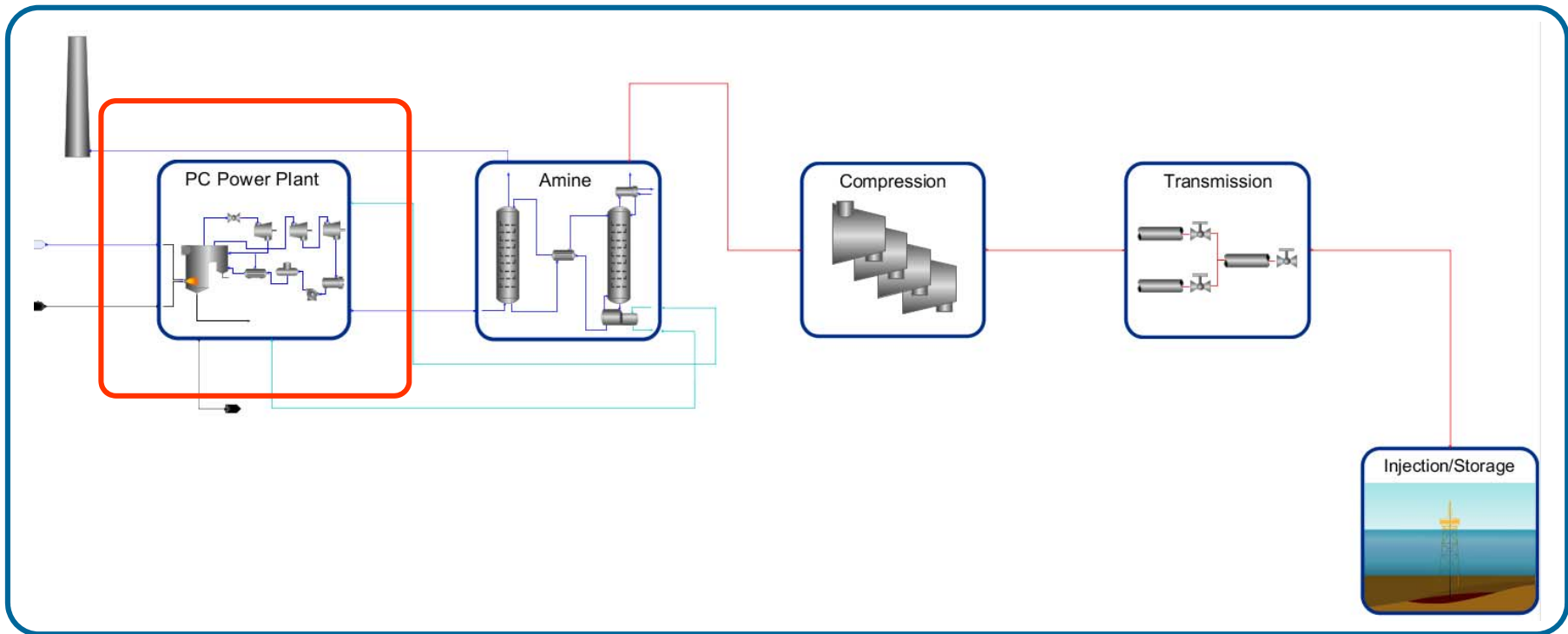
- Equipment CapEx & OpeX

■ Materials models

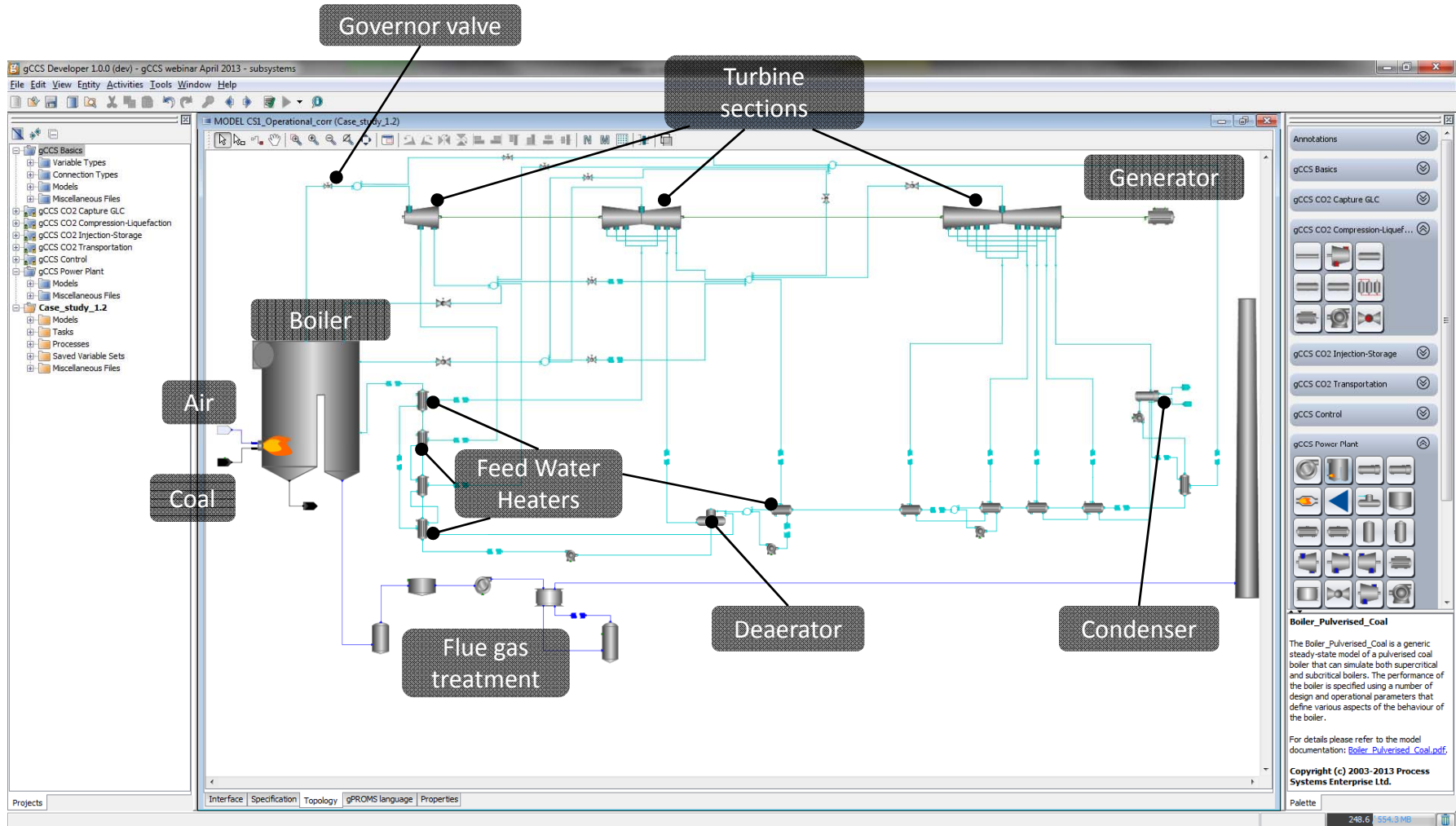
- cubic EoS (PR 78)
 - flue gas in power plant
- Corresponding States Model
 - water/steam streams
- SAFT-VR SW/ SAFT- γ Mie
 - solvent-containing streams in CO₂ capture
- SAFT- γ Mie
 - near-pure post-capture CO₂ streams

Open architecture allows incorporation of 3rd party models

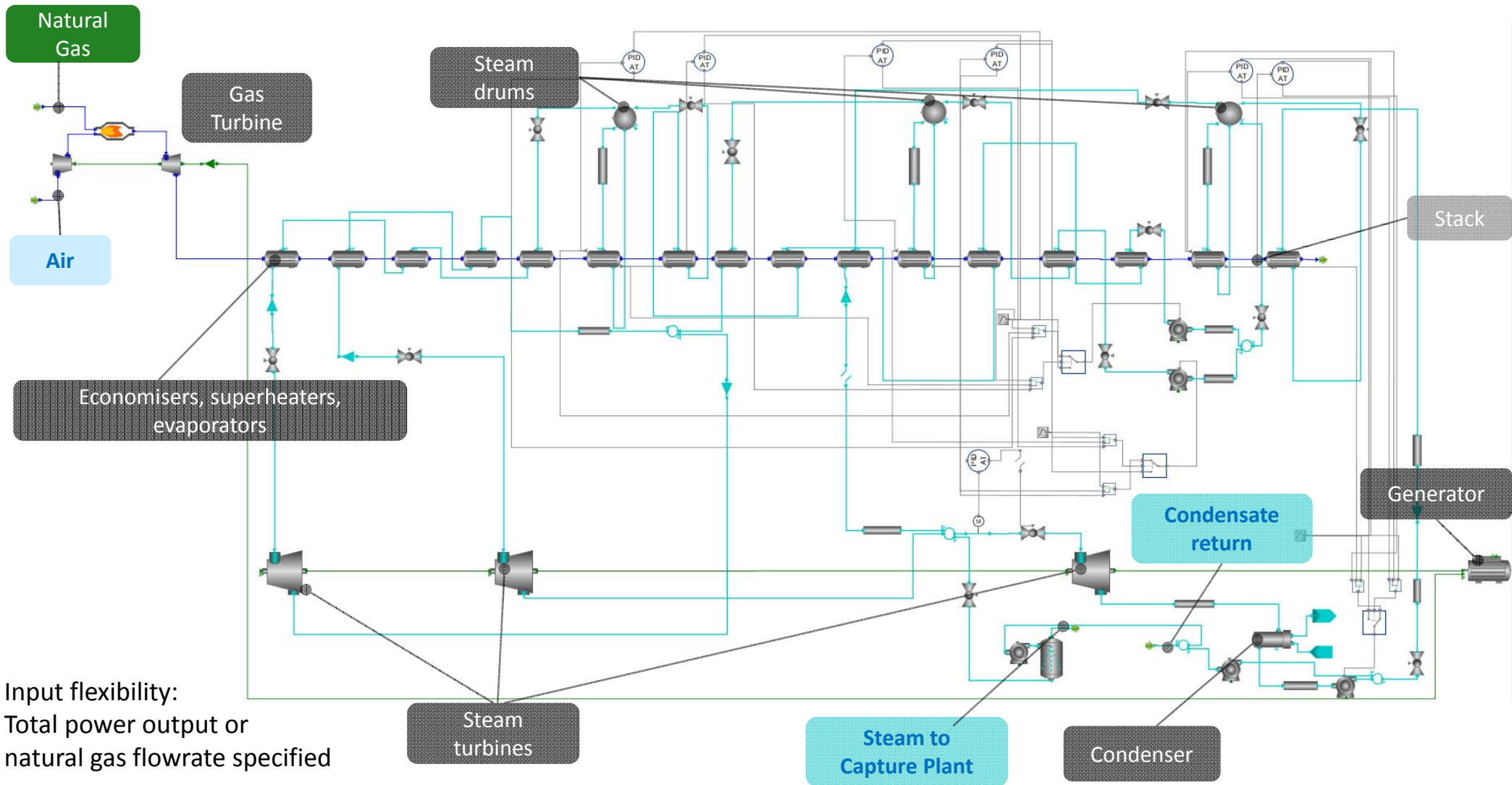
Power generation



gCCS Power Plant Library – conventional power generation Supercritical pulverized coal power plant



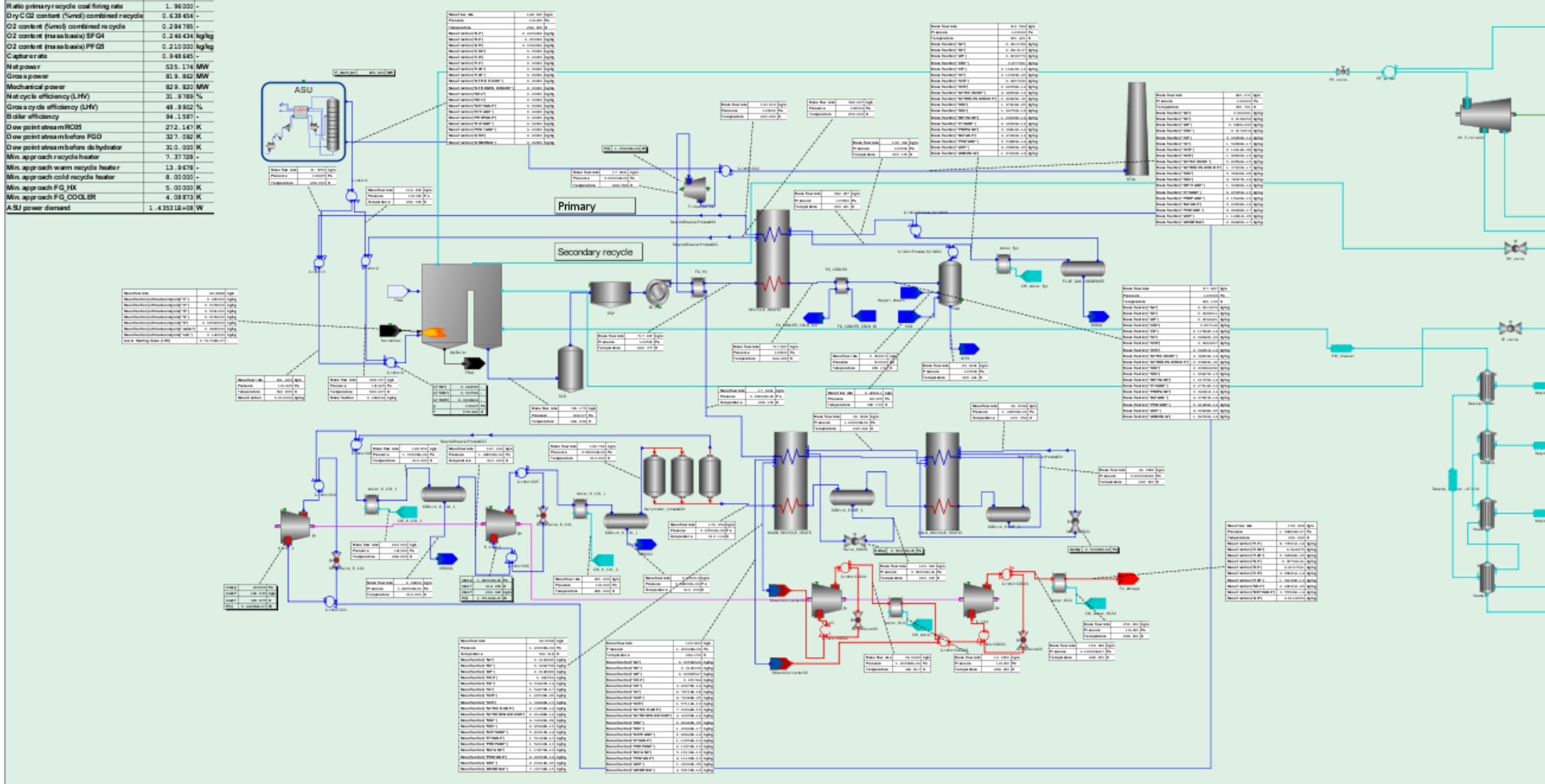
gCCS Power Plant library – conventional power generation NGCC power plant



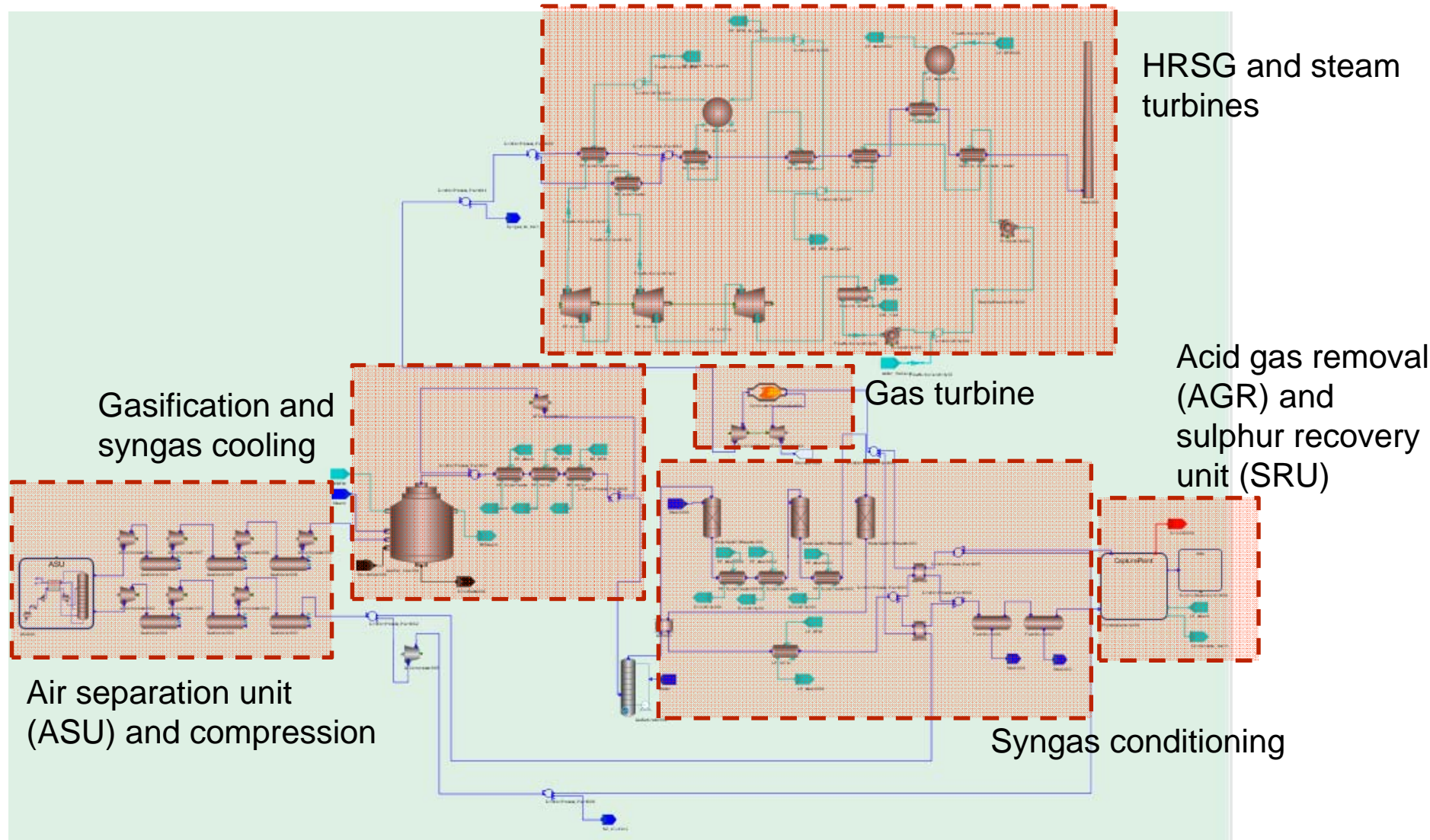
Oxyfuel system



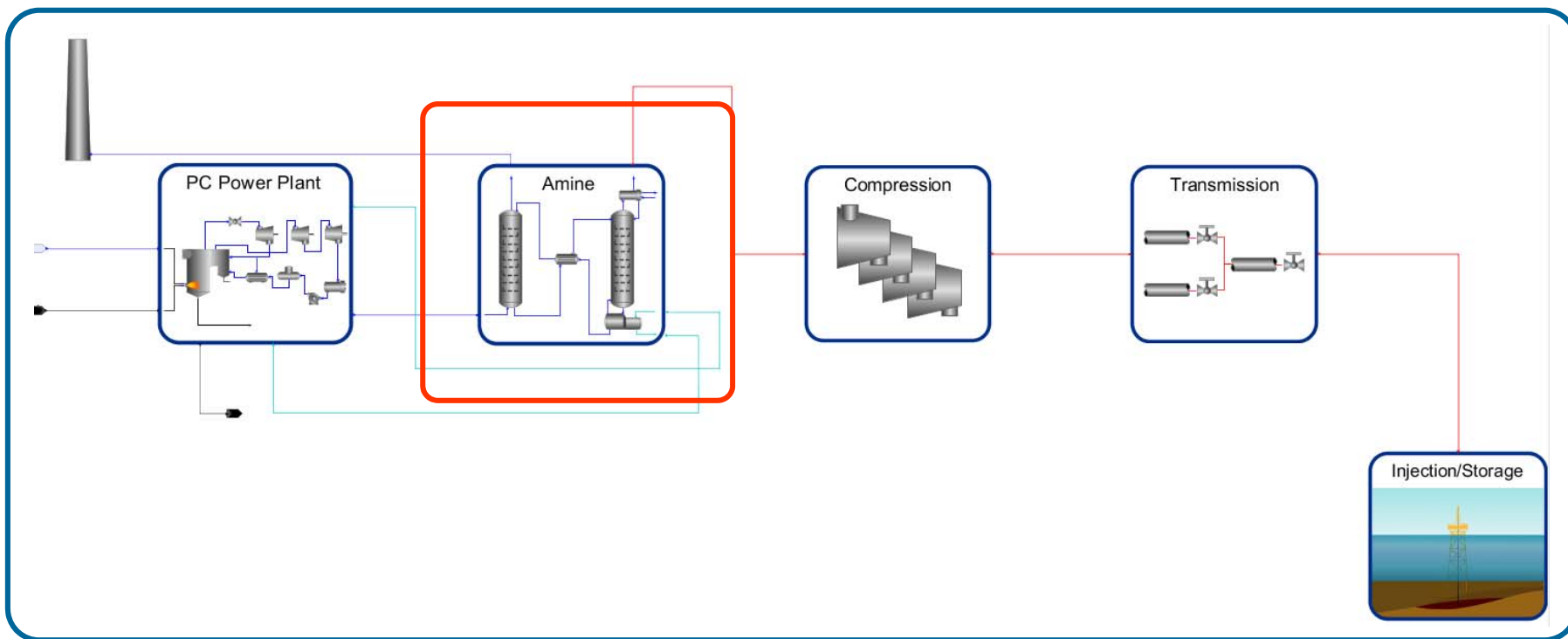
Total recycle ratio	0.740303	-
Ratio primary recycle coal firing rate	1.96303	-
Dry CO ₂ content (Nm ³) combined recycle	0.638454	-
O ₂ content (Nm ³) combined recycle	0.248793	-
O ₂ content (mass basis) SF G4	0.246434	kg/kg
O ₂ content (mass basis) SF G5	0.210303	kg/kg
Capex ratio	0.948443	-
Net power	535.174	MW
Gross power	819.962	MW
Mechanical power	829.820	MW
Net cycle efficiency (LHV)	31.9789	%
Gross cycle efficiency (LHV)	48.9902	%
Solar efficiency	34.1597	-
Dew point steam H2O5	273.147	K
Dew point steam before H2O2	327.326	K
Dew point steam before hydrator	310.003	K
Min. approach recycle heater	7.37328	-
Min. approach warm recycle heater	13.9478	-
Min. approach cold recycle heater	8.00303	-
Min. approach F.G. HX	15.00303	K
Min. approach F.G. COOLBR	4.08873	K
ASU power demand	1.43318+03	W



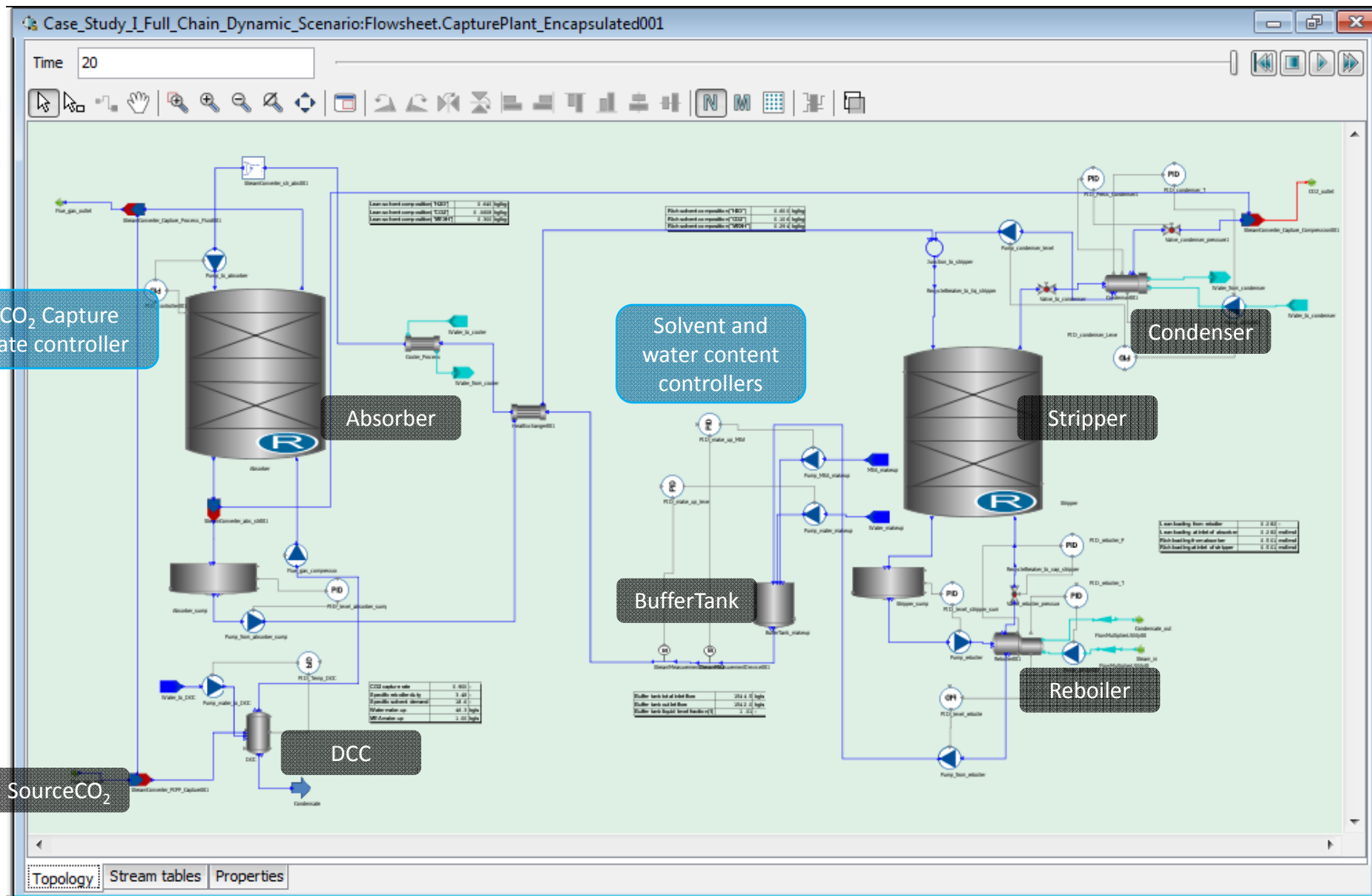
Integrated Gasification Combined Cycle (IGCC)

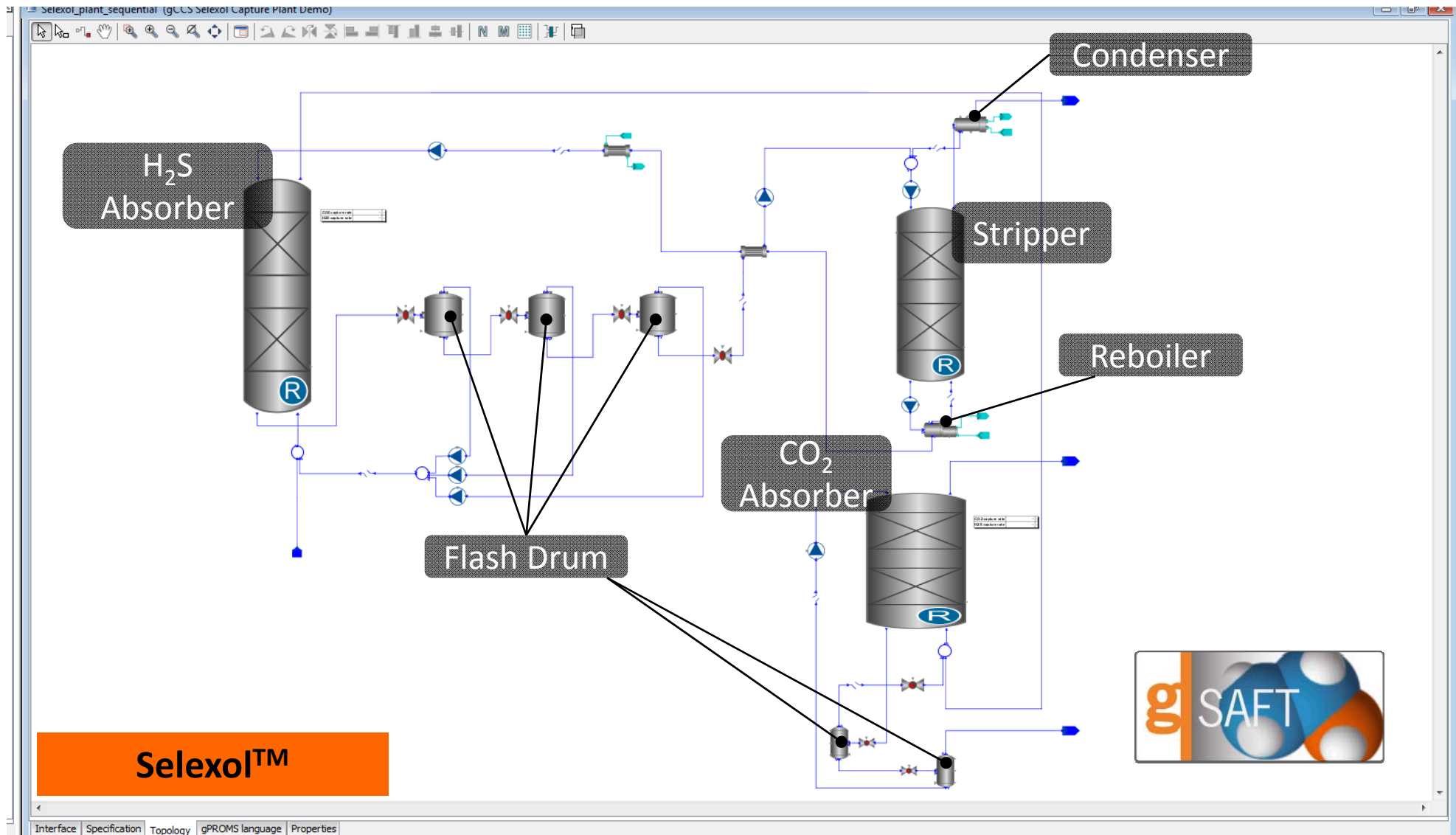


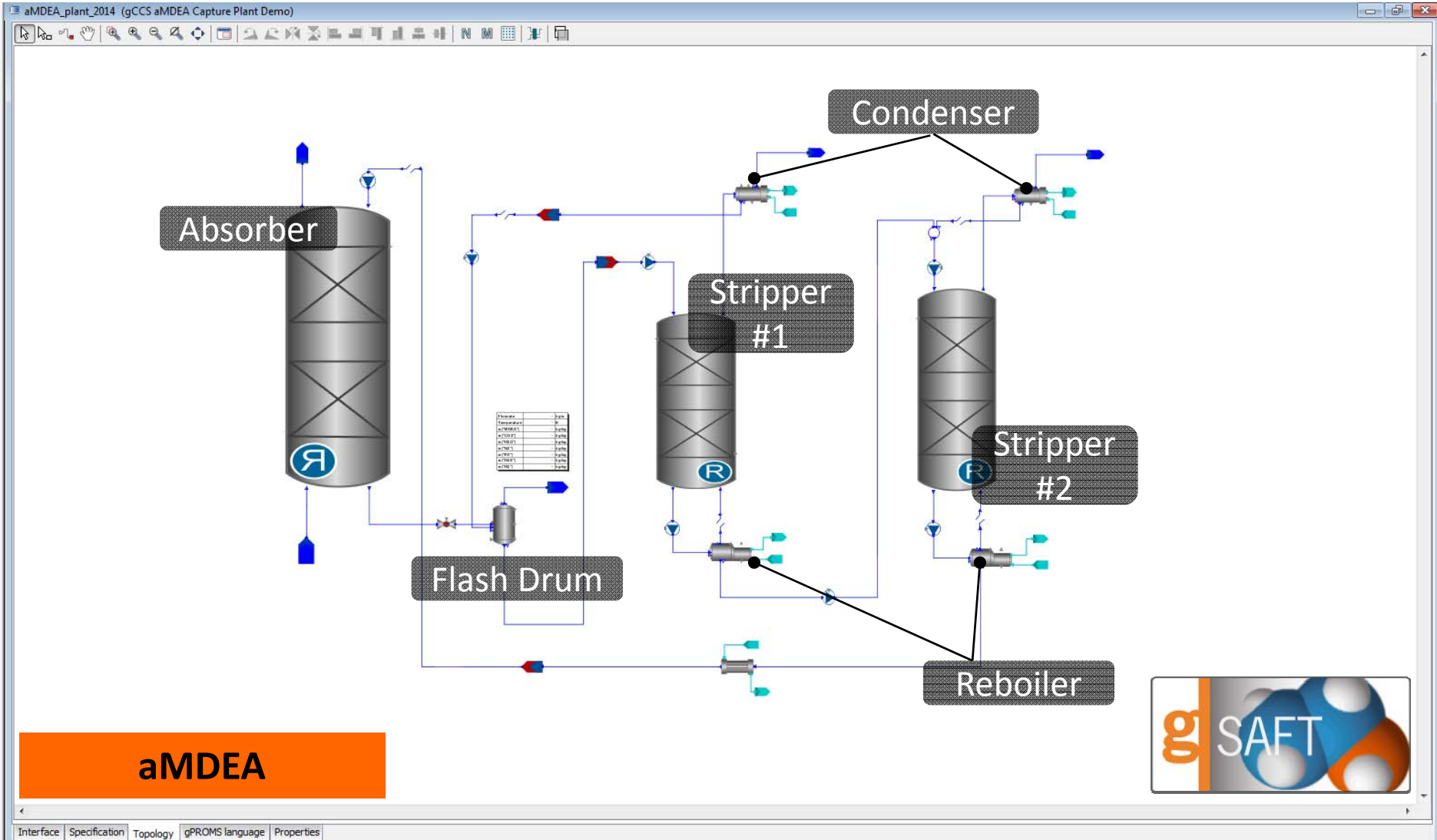
CO₂ Capture



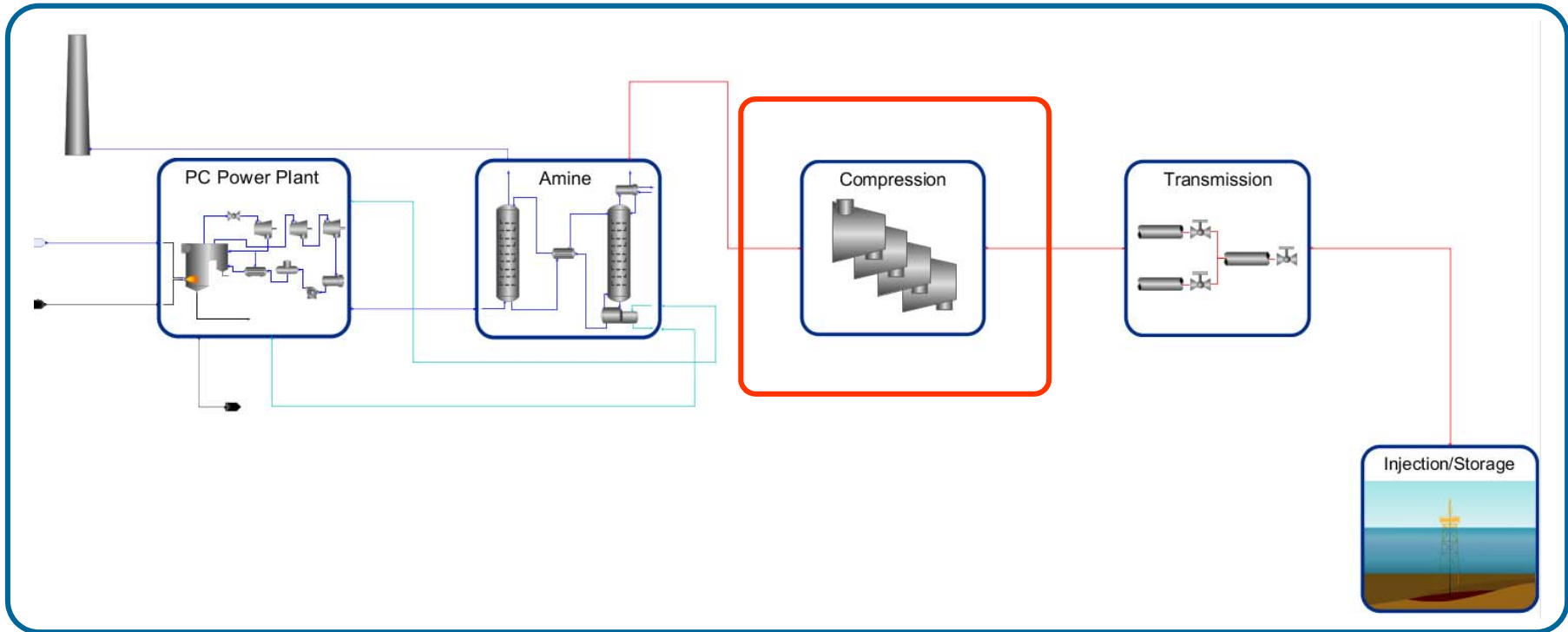
Chemical Absorption





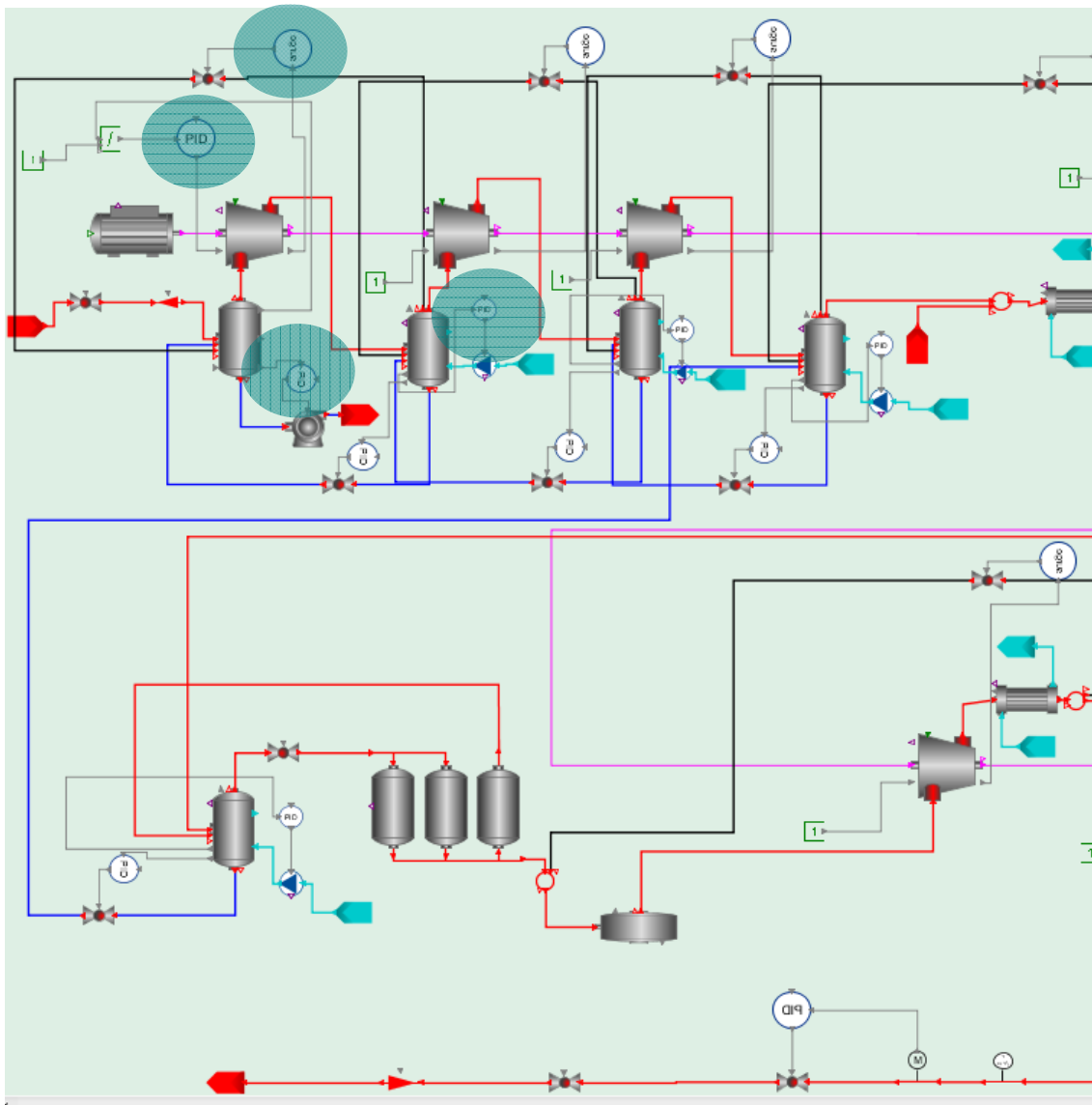


Compression



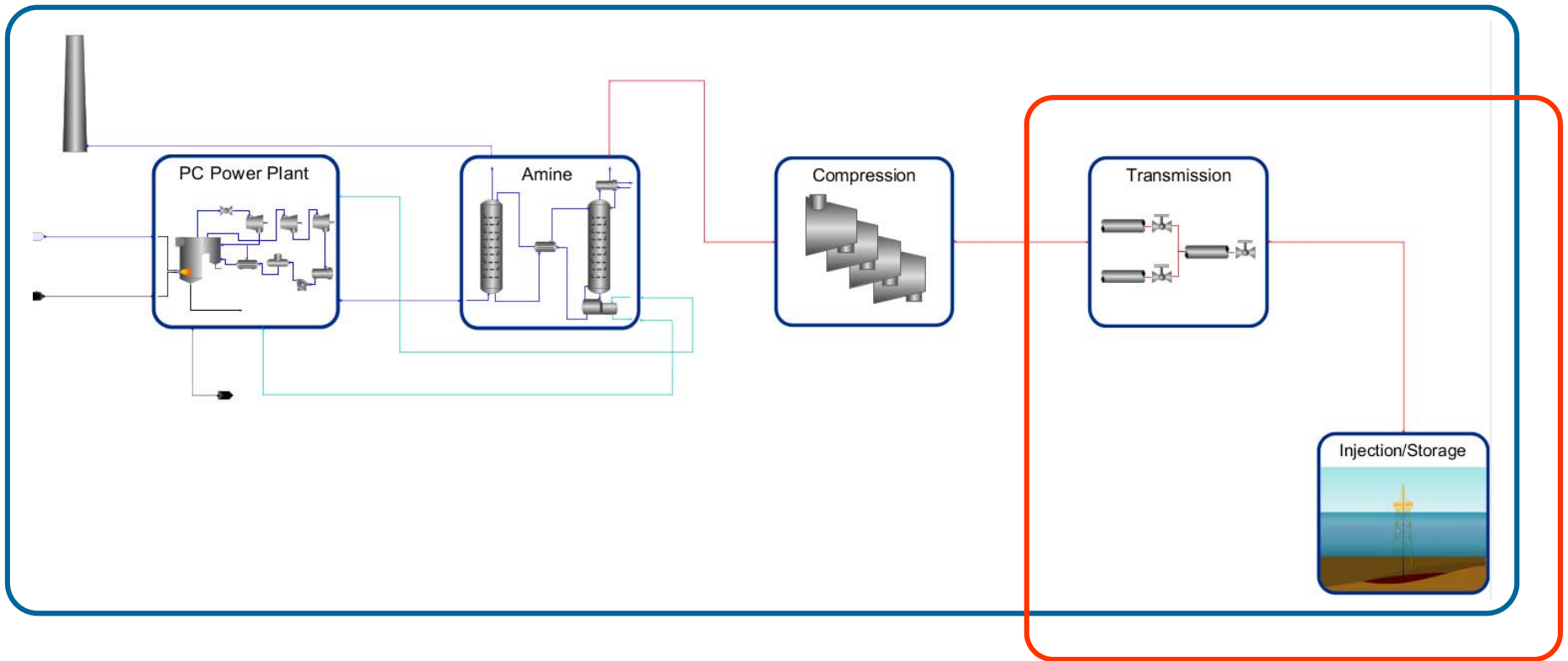
Multi-section compressor train

Including Control System

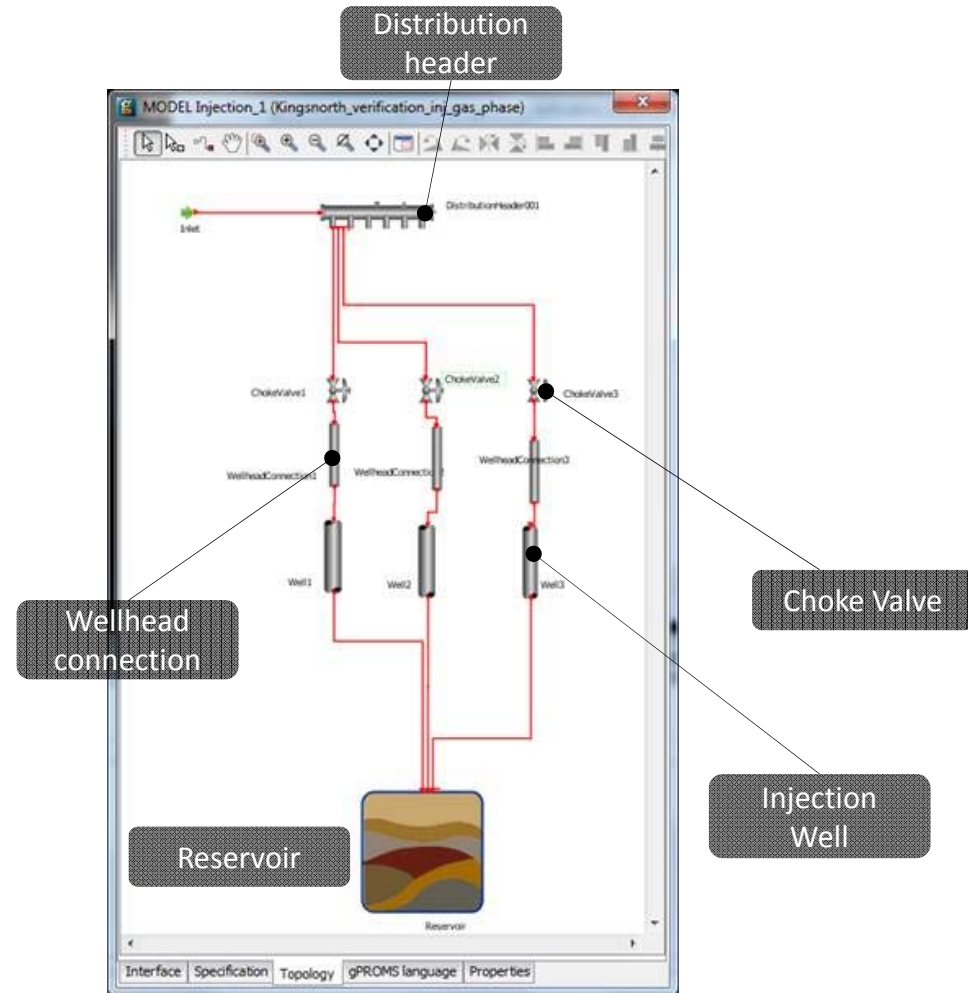
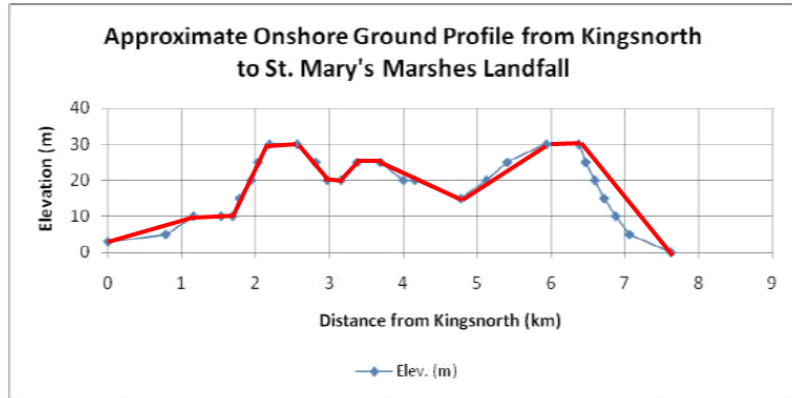
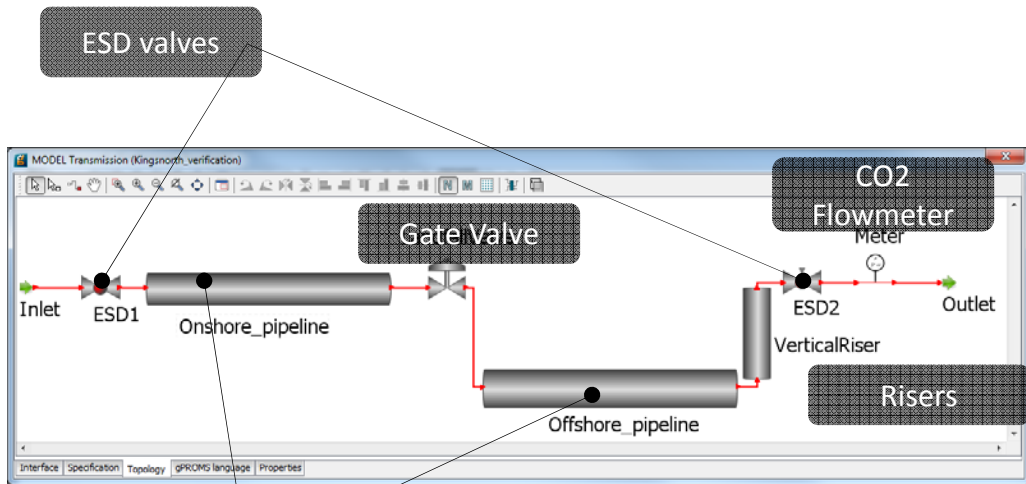


- Dynamics accounted for
 - KO-Drum mass/energy holdup
 - Shaft and compressor inertia
 - Valve dynamics
 - Opening time
 - Closing time
 - Controller parameters
- Suction pressure
 - IGV control
 - VFD control
- For every compression stage
 - Anti-surge control
 - Discharge temperature control
 - KO-Drum level control
- All safety valves
 - ESD valve
 - Check valve

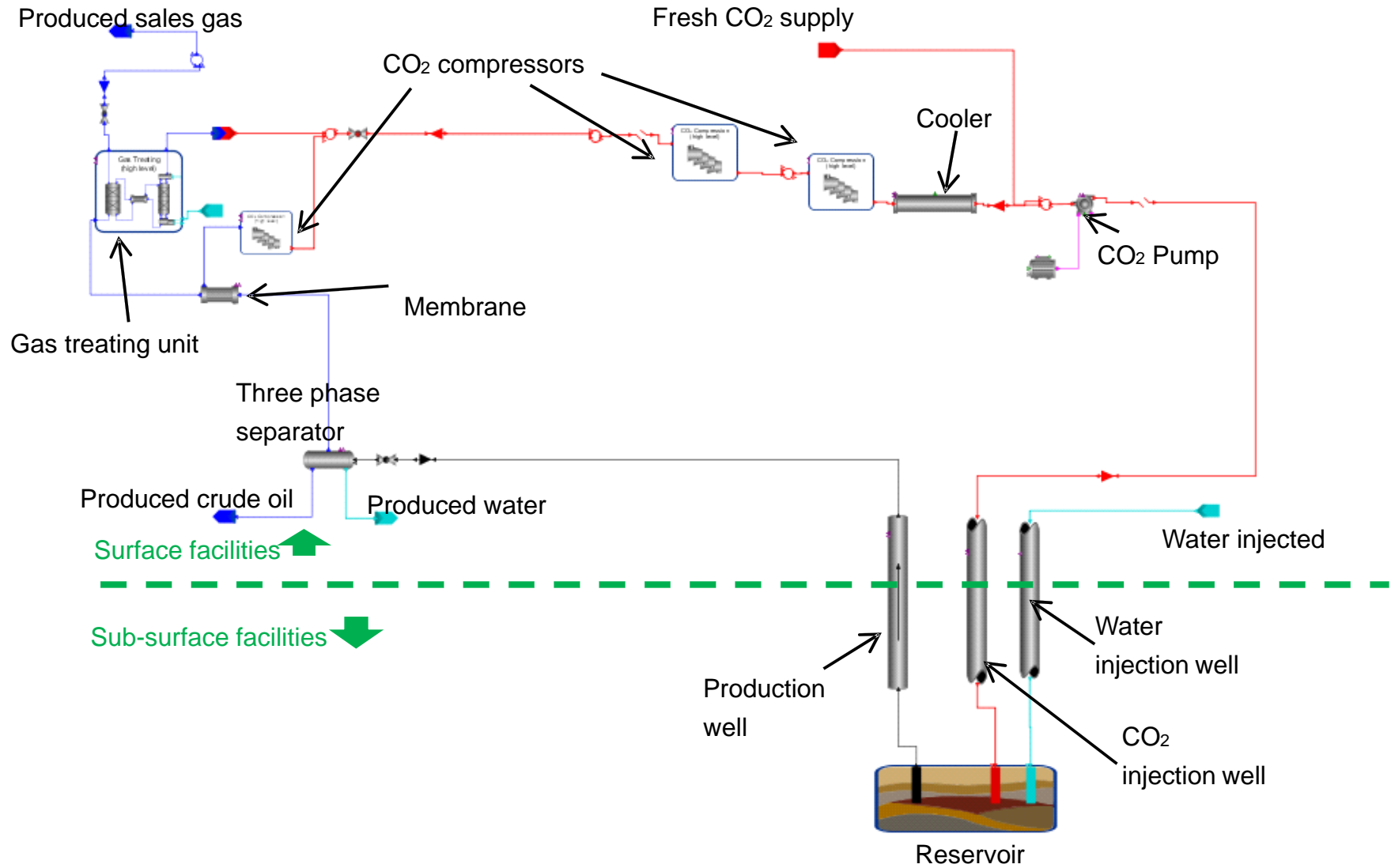
Transmission & injection



Transmission and Injection



CO₂ Enhanced Oil Recovery



Applications of gCCS: Case Studies

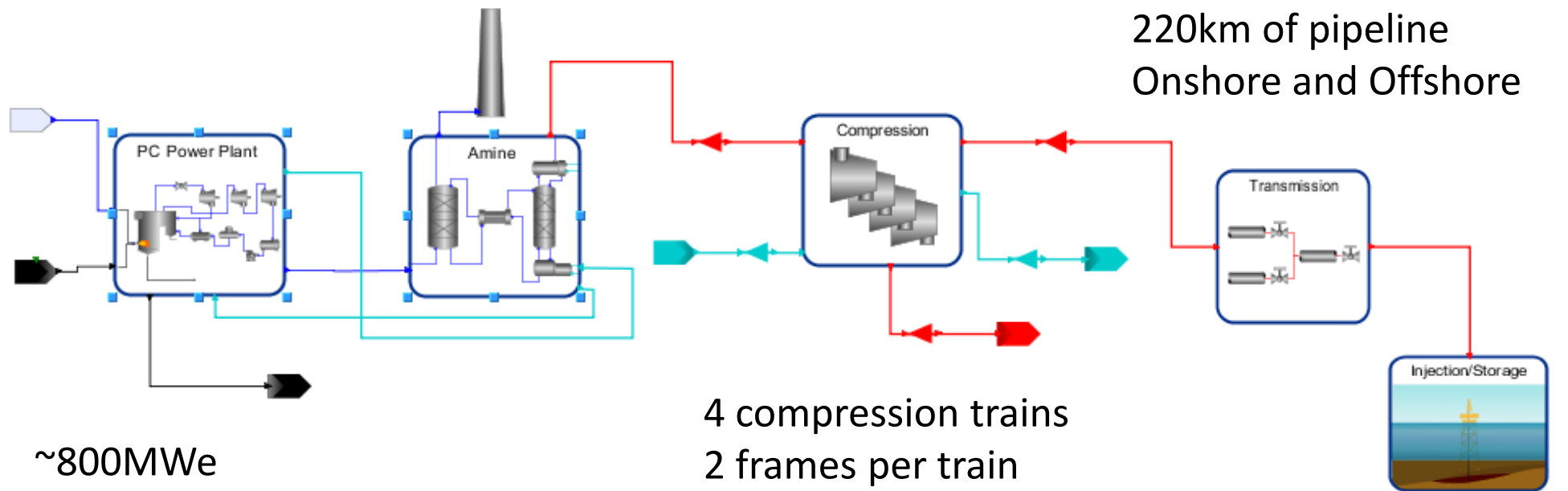


1. Process integration in CCS chains and networks

CCS Chain model developed in gCCS



Chemical absorption
MEA solvent
90% CO₂ capture



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

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

220km of pipeline
Onshore and Offshore

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

Steady-state scenarios



Scenario	Description	Power plant operation (% of nominal load)	Capture plant operation (CO2 % captured)
SS1.1 (a,b,c)	Base Load Power Plant	(a) 100%; (b) 75%; (c) 50%	0% (no capture)
SS1.2 (a, b)	Base load CCS Chain	100%	(a) 90%; (b) 50%
SS1.3 (a, b)	Part Load Analysis	(a) 75%; (b) 50%	90%
SS1.4	Extreme Weather: Max Summer	100%	90%
SS1.5	Extreme Weather: Min Winter	100%	90%

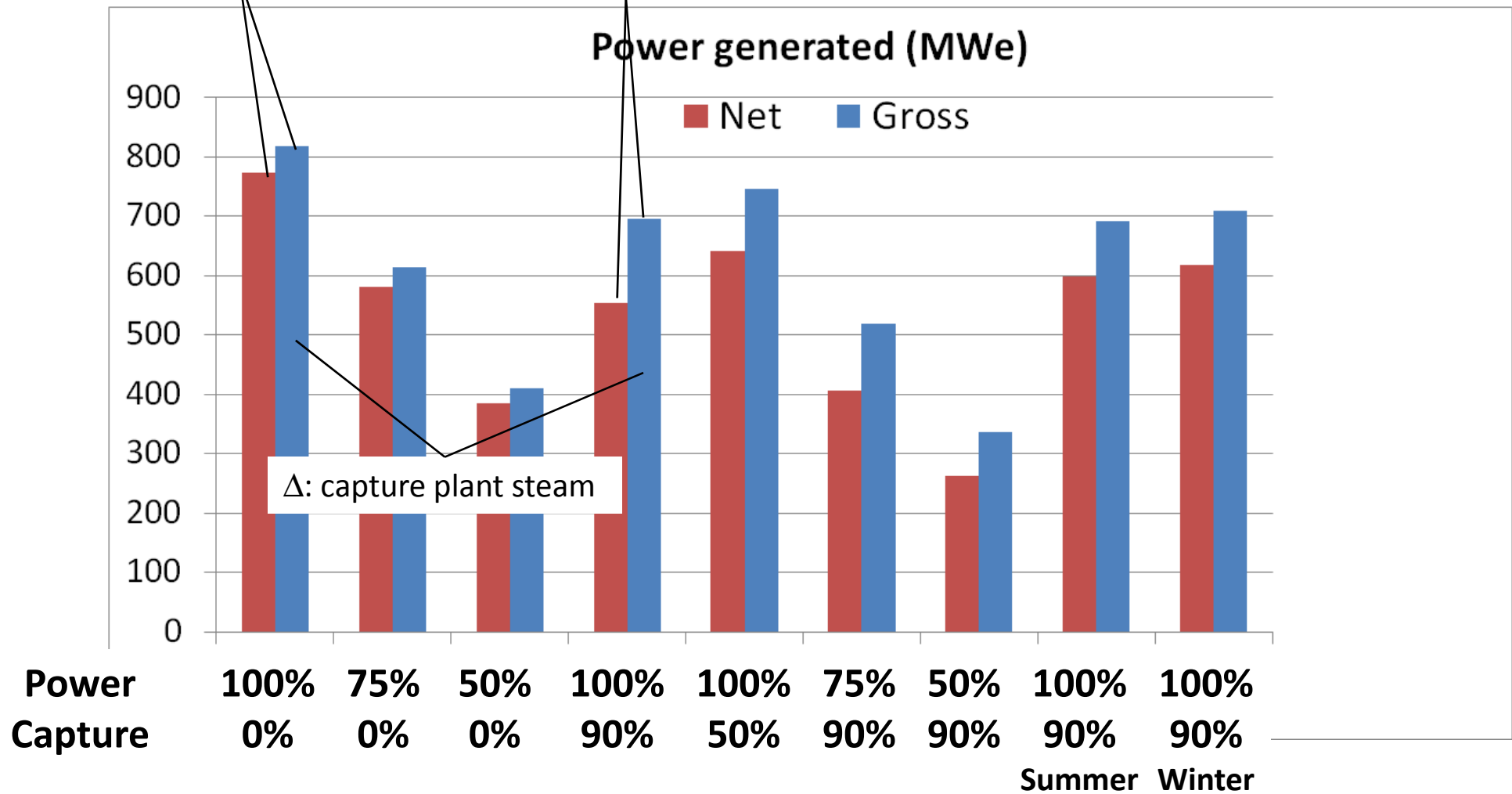
Temperatures (°C)	Affected sub-systems	Base Case	Extreme Summer	Extreme Winter
Cooling water	Power, Capture, Compression	18	22	7
Air	Power, Transmission, Injection	15	30	-15
Sea water	Transmission, Injection	9	14	4
NB. Geothermal gradient of +27.5°C / km				

Steady-state analysis

Power generation



Δ : coal milling
 + power plant auxiliaries
 Δ : coal milling
 + power plant auxiliaries
 + CO₂ compression

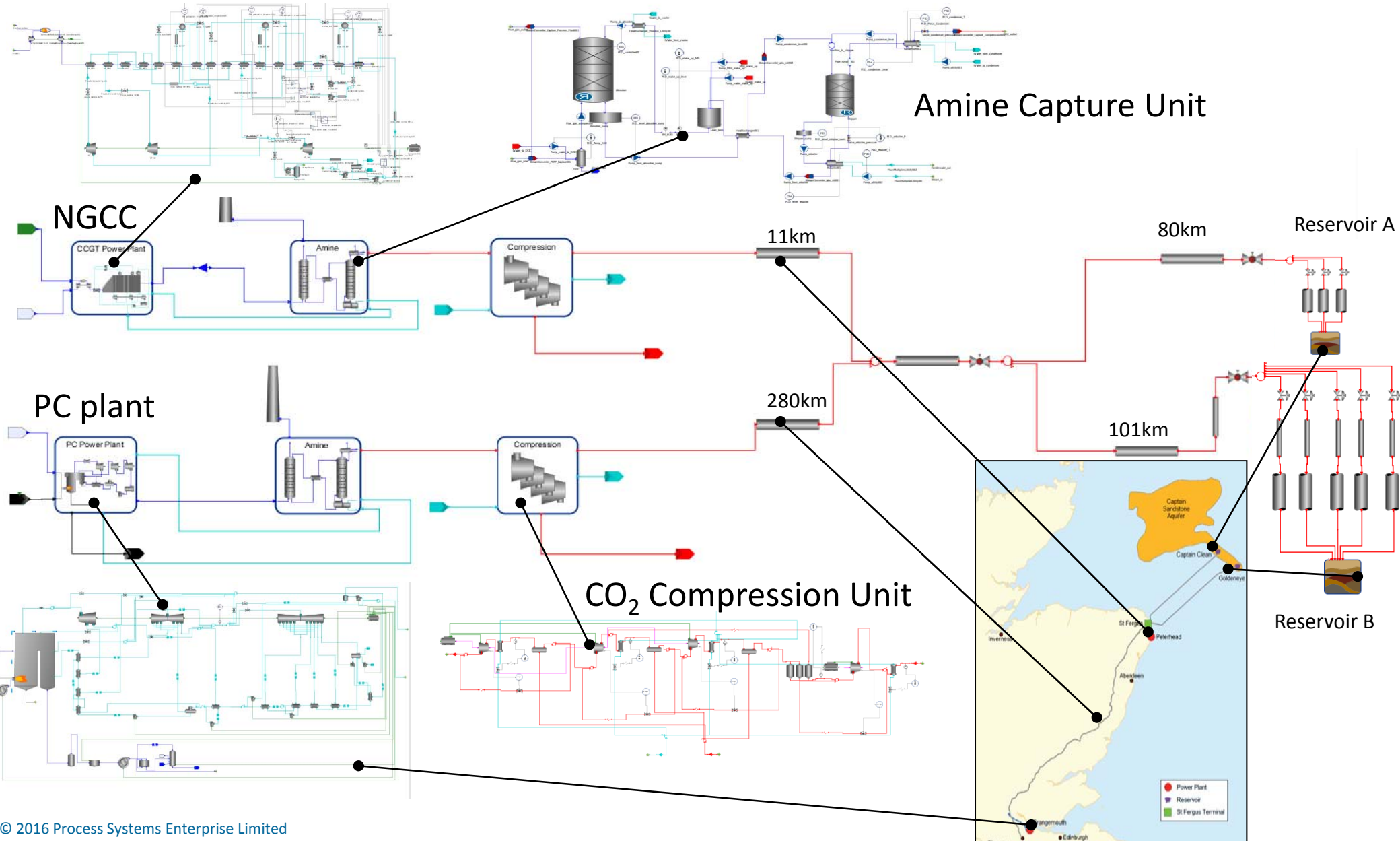


Applications of gCCS: Case Studies



2. Dynamics in CCS Networks

CCS network modelling in gCCS

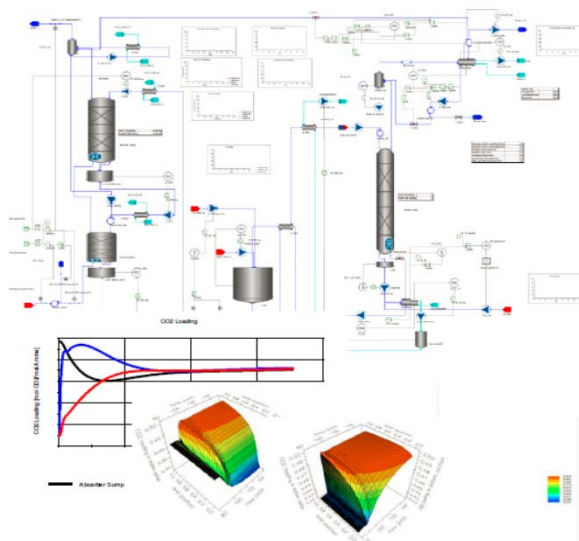
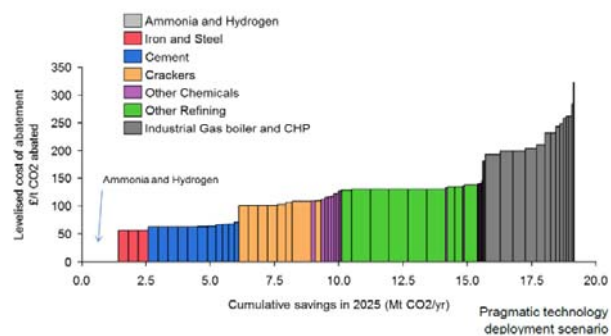


Industrial projects

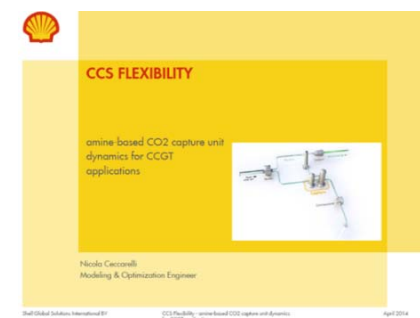


Techno-economic study of Industrial Carbon Capture and storage [DECC and Element Energy]

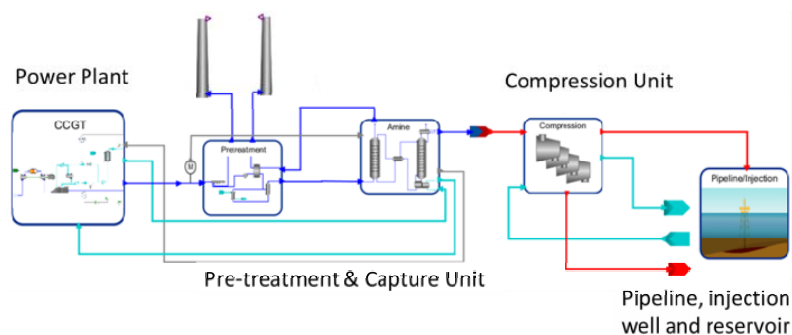
MACC curve of capture technologies



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



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



Status update and next steps

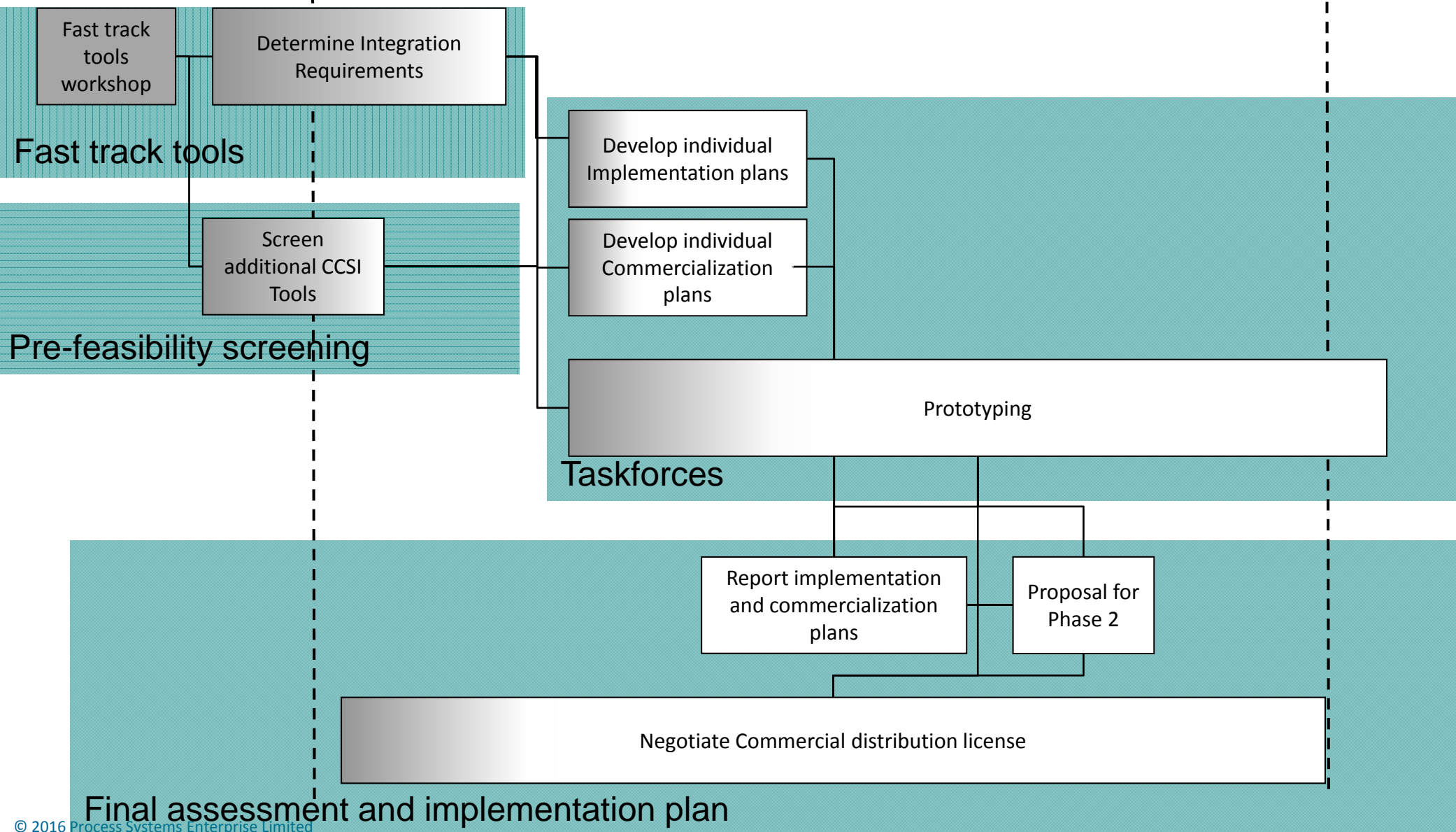


Project overview and status update

Project structure



2015 | 2016 | 2017



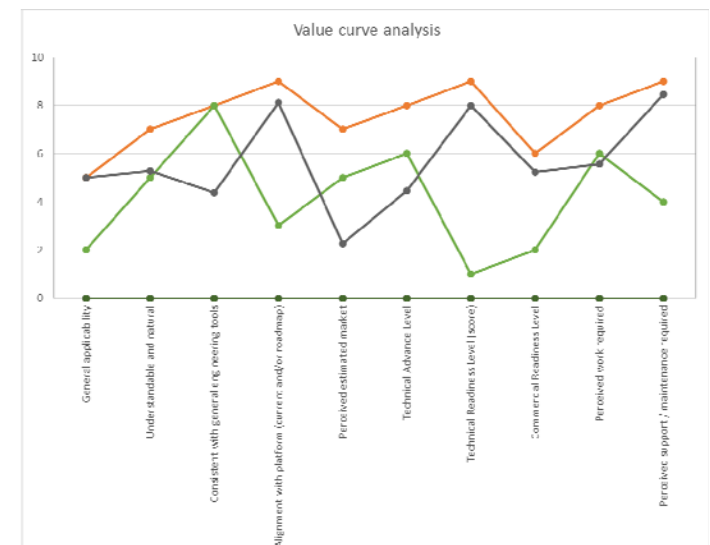
Current status



- Completed recruitment of new resources
- Completed Workshops for fast-tracked CCSI tools
- Defined sub-projects for WVU and CMU
- Developed screening criteria and commenced with screening other CCSI tools
- Ongoing negotiations of commercial licenses
- Ongoing familiarization exercises with CCSI toolkit

Screening spreadsheet

The screenshot shows a spreadsheet with columns for various criteria and rows for different projects or tools. The criteria include 'Market', 'Market score', 'Competitors', 'Barriers to entry (i.e. ease of market break gain)', and 'First mover advantage'. The data is represented by colored cells (green, yellow, red) and numerical values.

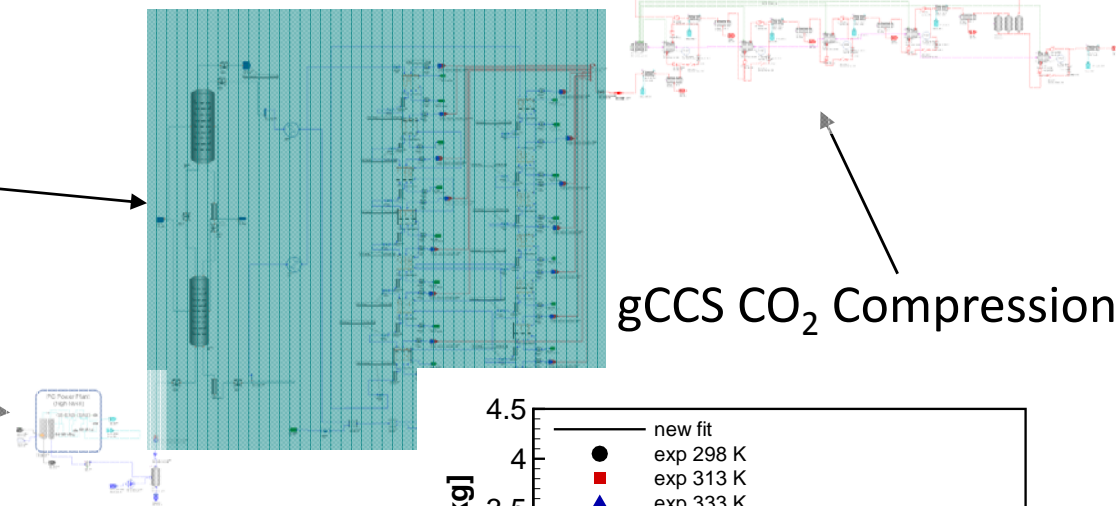


- ALAMO being used to generate a property method model from property model data
- Prototype interfaces between ALAMO and gPROMS in development
- ALAMO brochure developed describing
 - Workflow
 - Potential applications
 - Competitors
 - SWOT Analysis
- Market research carried out

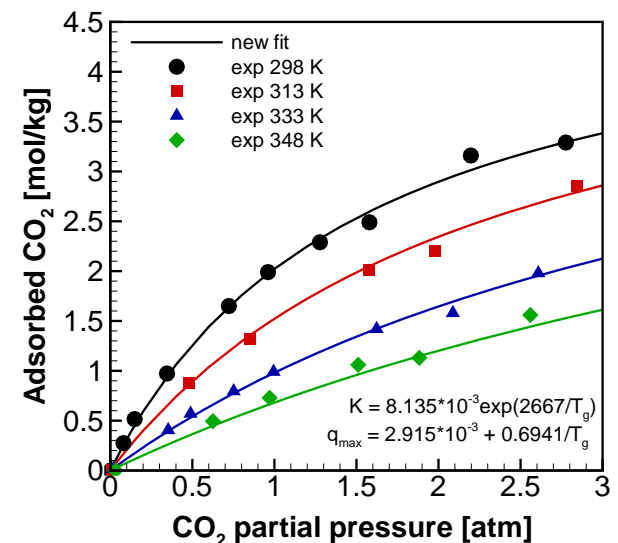
- CCSI tools consist of flowsheets with Bubbling fluidized bed (BFB) and Moving bed (MB) models
- This was integrated with other gCCS models

CCSI BFB and MB models

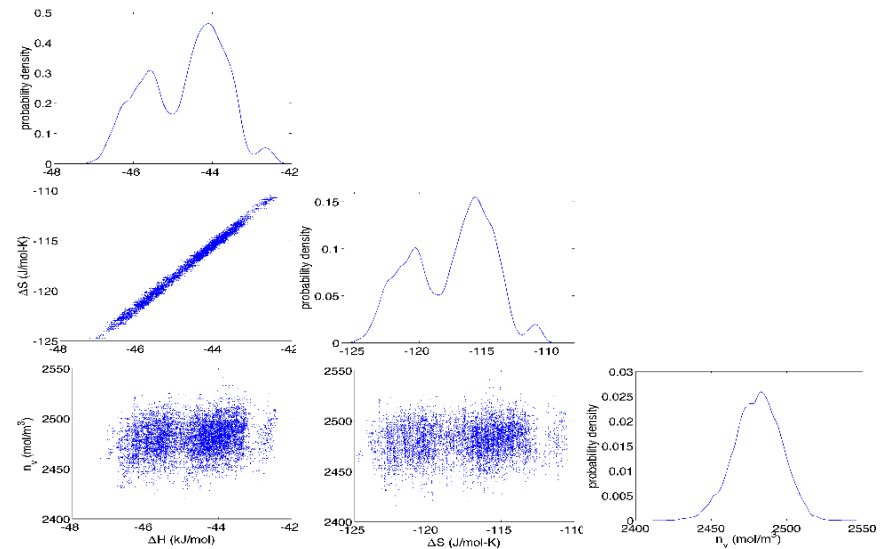
gCCS Power plant



- A fixed bed adsorber model was developed to extend the model library
- Market research activities carried out
- Brochure developed



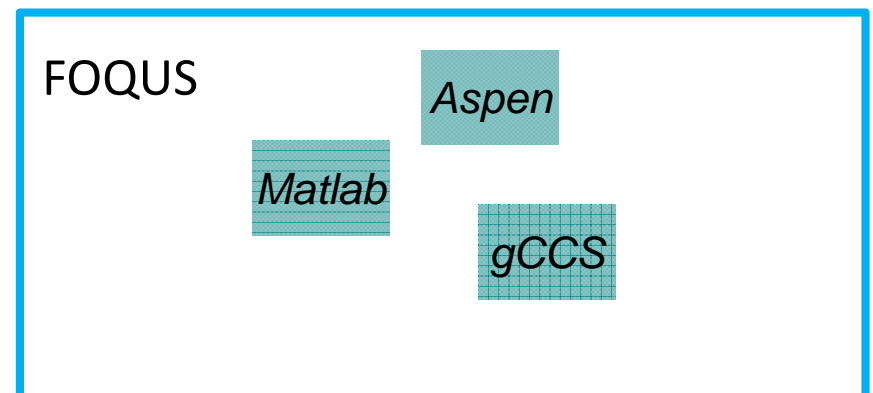
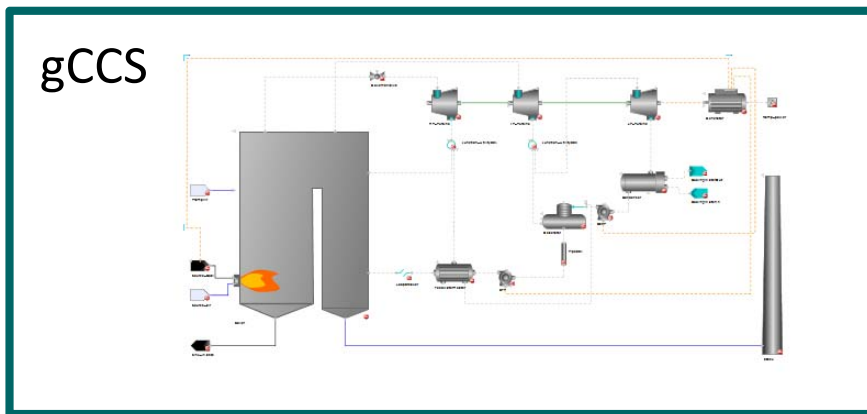
- Fits combined thermodynamic and kinetic models of amine-based CO₂ solid sorbents to lab/bench-scale data
- Demonstrated the uncertainty quantification features of the tool
- Prototype interfaces between SorbentFit and gPROMS in development
- Brochure in development



FOQUS Flowsheet + SimSinter



- SimSinter provides a wrapper to enable models created in process simulators to be linked into a FOQUS Flowsheet
- Brochure in development



Summary



- Advanced process modelling is an essential tool
 - inform and aid the **design** of CCS systems and network and **reduce capital expenditure** of large-scale integrated CCS projects
 - Minimise **operating expenditure** by integrating **dynamic operation** and considering **scale** aspects
 - **Evaluate technology** – benchmarking existing and provide a basis to **assess** budding **next-generation technology**
- **Transfer** experience and best-practice between demonstration and large-scale integrated CCS projects
- **Integrating platform** for working with other stakeholders in chain collaborative R&D, working with academia

Next steps for the next period



- Complete screening for non-fast-track tools
- Set up discussions with members of Industrial Advisory Board to help prioritise screening process
- Assess of integration requirements for fast-track tools

Improving commercial viability and reducing technology risk



■ Business case

- Reduce cost (particularly CapEx)
- Understand financial risk to investors
- Support negotiations between emitters and ‘carbon uptakers’
- Assess impact of various trip scenarios on generated ‘clean electricity’ (and thus, price of electricity)

■ Flexibility of CCS Systems

- Start-up/shut-down sequences
- How fast can the capture unit be ramped down with load?

■ Safety analysis

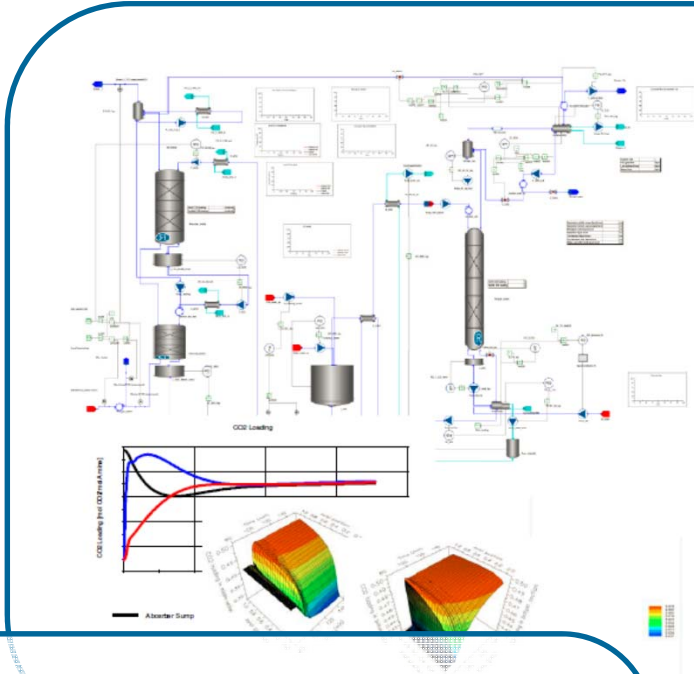
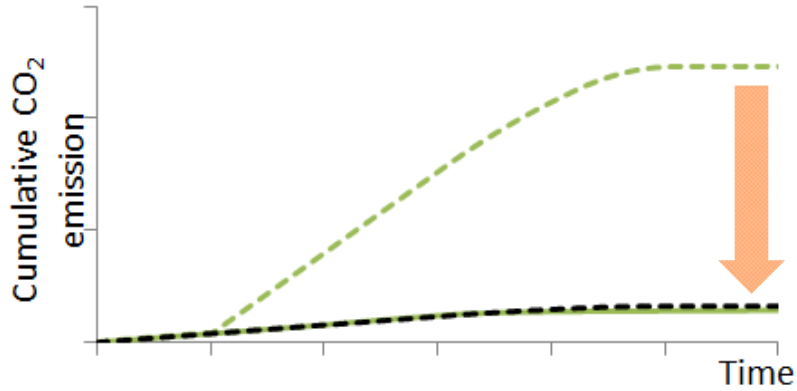
- Assess impact of turbine/compressor/injection trips
- Quantify reaction time available along the CCS chain depending on a specific trip scenario

Thank you

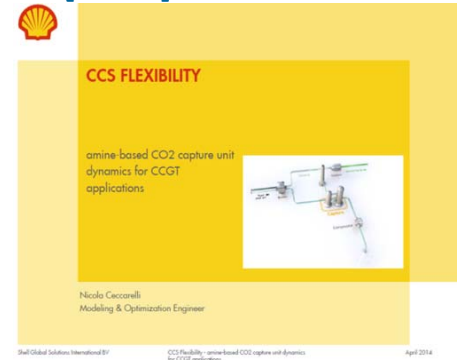


Industrial and UK Government-funded projects

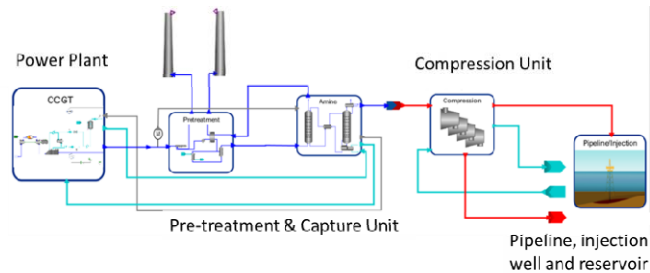
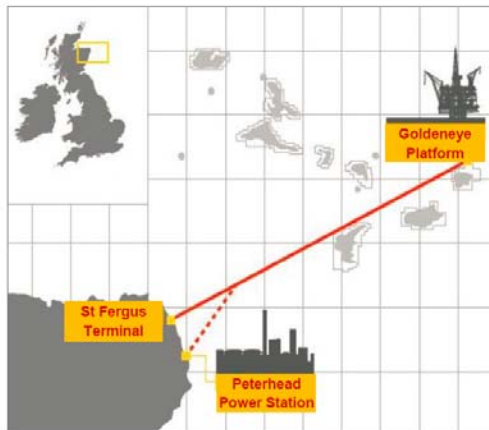




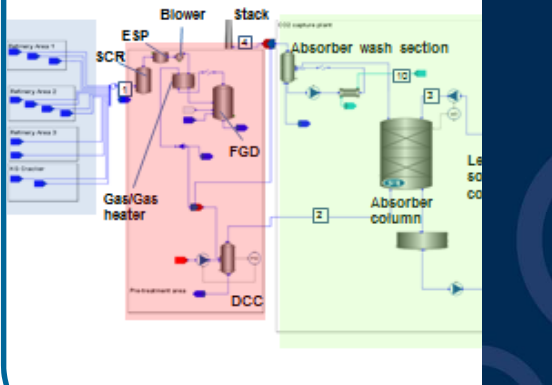
Optimizing start-up and shutdown procedures of gas treating plants [Shell]



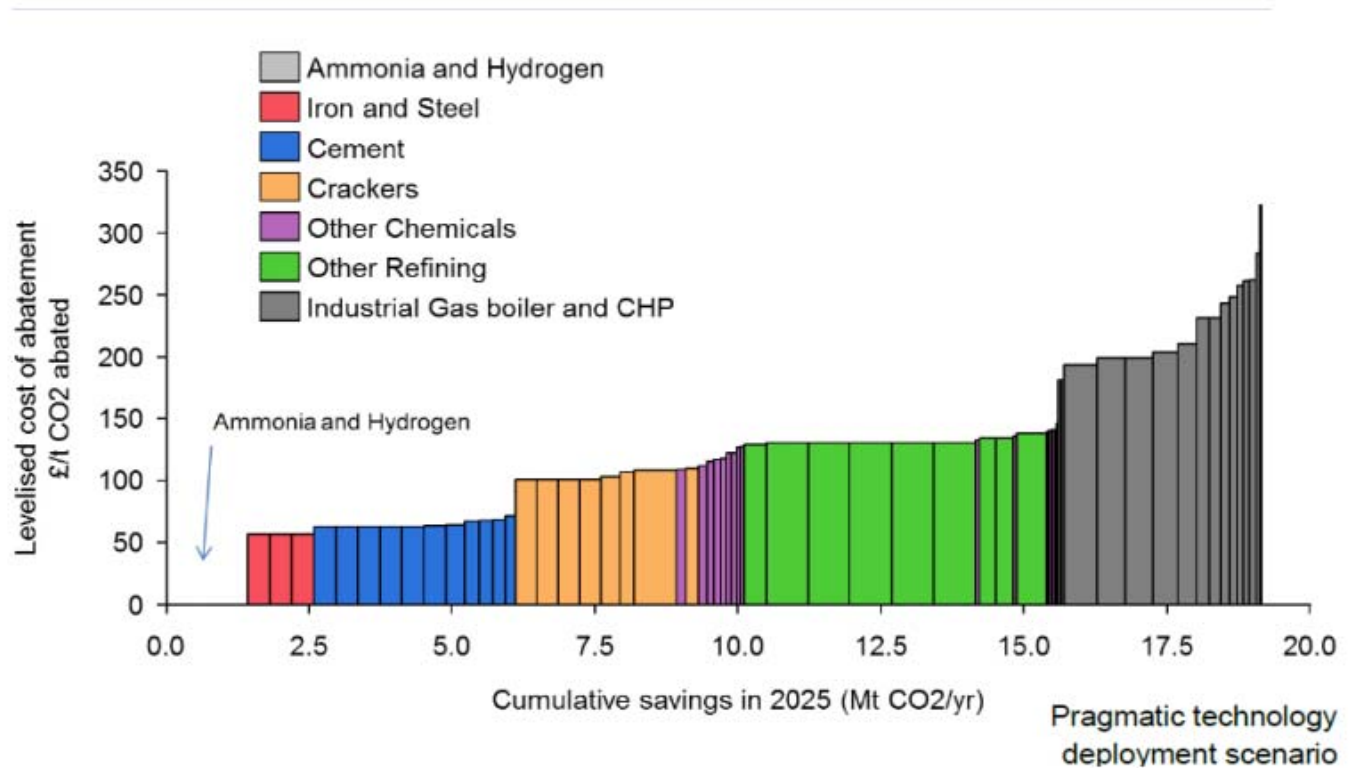
CCS chain and network studies [Energy Technologies Institute] and [Shell]



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



MACC curve of capture technologies



Specific Project Objectives

- Reduce the solvent regeneration energy footprint by up to 40% as compared to a standard/current MEA process.
- Demonstrate zero solvent emissions from carbon capture plant.
- Reduce corrosion rates to migrate to inexpensive material of construction.
- Focus on process standardization, intensification and industrial scale up. Reduce the overall level of plant redundancy and overdesign to account for outage and performance risks in the future CO₂ capture systems.
- **Development of high-fidelity predictive models for optimising the design and operation of the full-scale plant in order to realise the full extent of these savings.**



Department
of Energy &
Climate Change

Benefits

- The novel APBS solvents reduce the steam consumption by up to 40% which translates to an approximate 22% reduction in LCOE (levelised cost of electricity) for a CCS enabled power plant.
- Auxiliary electrical load, which consists mainly of pumps and fans, can be reduced by 50%.
- Improved process layout, which maximizes sharing of infrastructures and mitigation of expensive connections.
- Process standardization, better layouts and best metering technology selection will boost the confidence in future leading to savings realization between 5% - 7%. Also reduced redundancy and overdesign will reduce the risk premium leading to savings between 2% - 4%.

■ Process models

- Power generation
 - Conventional:
pulverised-coal, CCGT
 - Non-conventional:
oxy-fuelled, IGCC
- Solvent-based CO₂ capture
- CO₂ compression & liquefaction
- CO₂ transportation
- CO₂ injection in sub-sea storage

■ Materials models

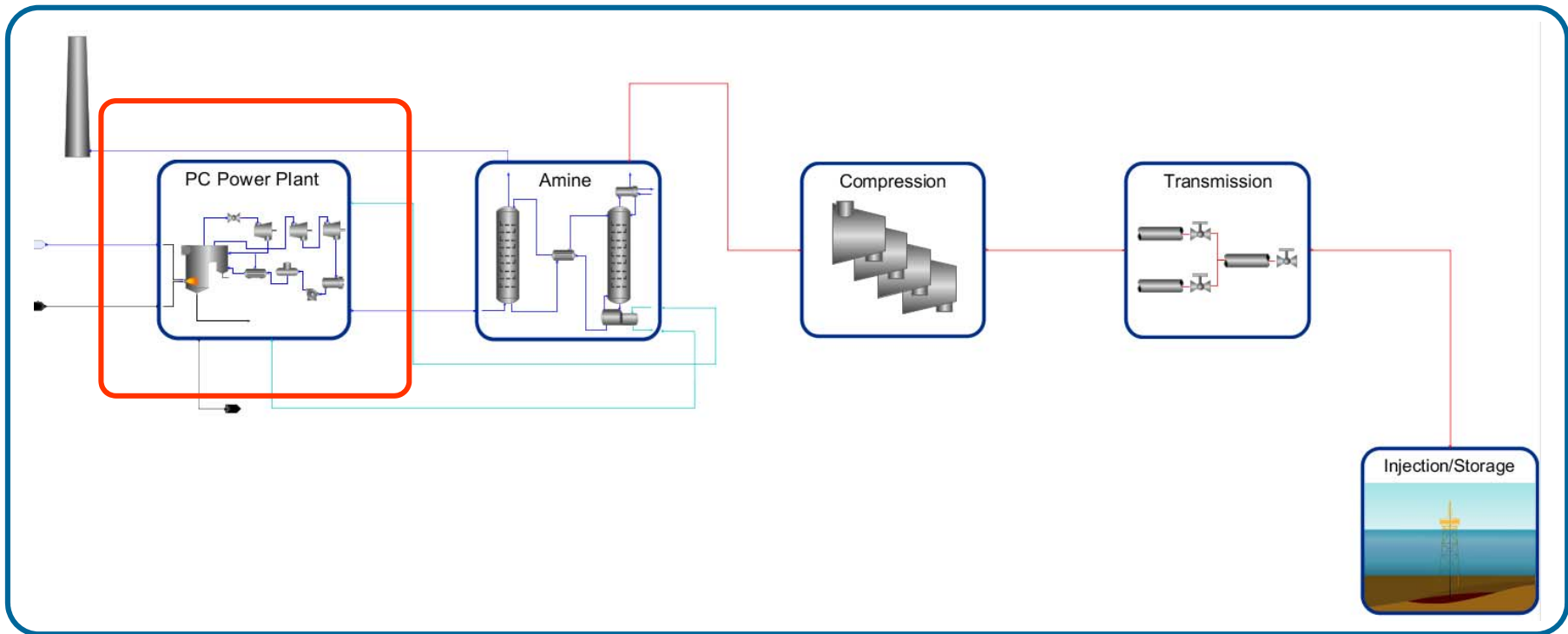
- cubic EoS (PR 78)
 - flue gas in power plant
- Corresponding States Model
 - water/steam streams
- SAFT-VR SW/ SAFT- γ Mie
 - solvent-containing streams in CO₂ capture
- SAFT- γ Mie
 - near-pure post-capture CO₂ streams

Toolkit Graphical User Interface

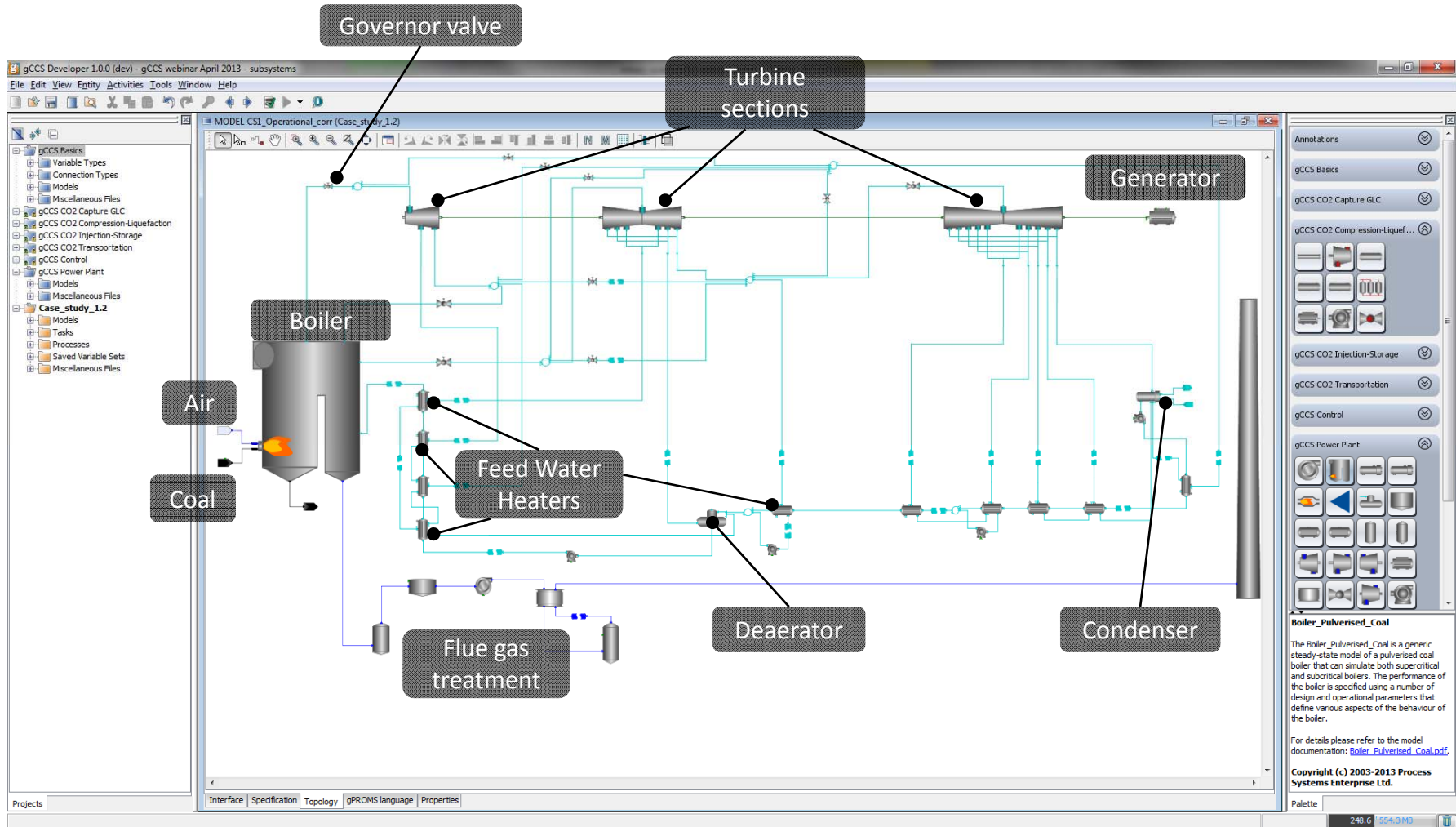


The screenshot displays the gCCS Developer 1.0.0 (dev) software interface. The main workspace is filled with a detailed process flow diagram for a CO2 capture and transport system. The diagram includes several interconnected units: a PC Power Plant, Amine scrubbers, a Compression section with multiple compressor stages, a Transmission pipeline, and an Injection/Storage reservoir. The interface is organized into several windows, each showing a different view of the process: 'Topology', 'Stream tables', and 'Properties'. A central 'Injection/Storage' window shows a 3D visualization of a wellhead in a reservoir. On the right side, there is a 'Palette' containing various components categorized under 'gCCS Basics', 'gCCS CO2 Capture', 'gCCS CO2 Compression-Liquefaction', 'gCCS CO2 Injection-Storage', 'gCCS CO2 Transportation', 'gCCS Control', and 'gCCS Power Plant'. The bottom status bar indicates '206.2 / 331.8 MB'.

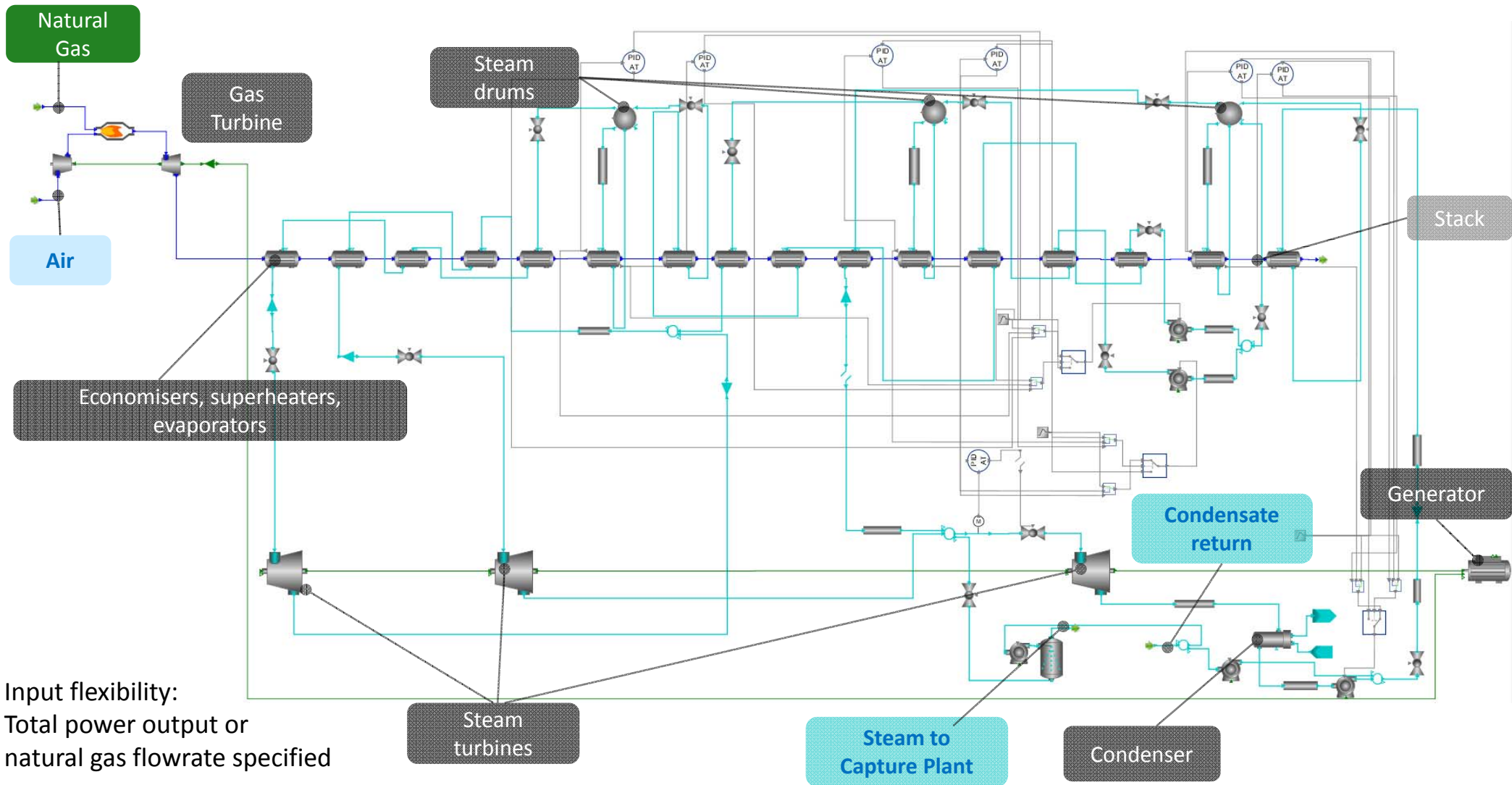
Power generation



gCCS Power Plant Library – conventional power generation Supercritical pulverized coal power plant



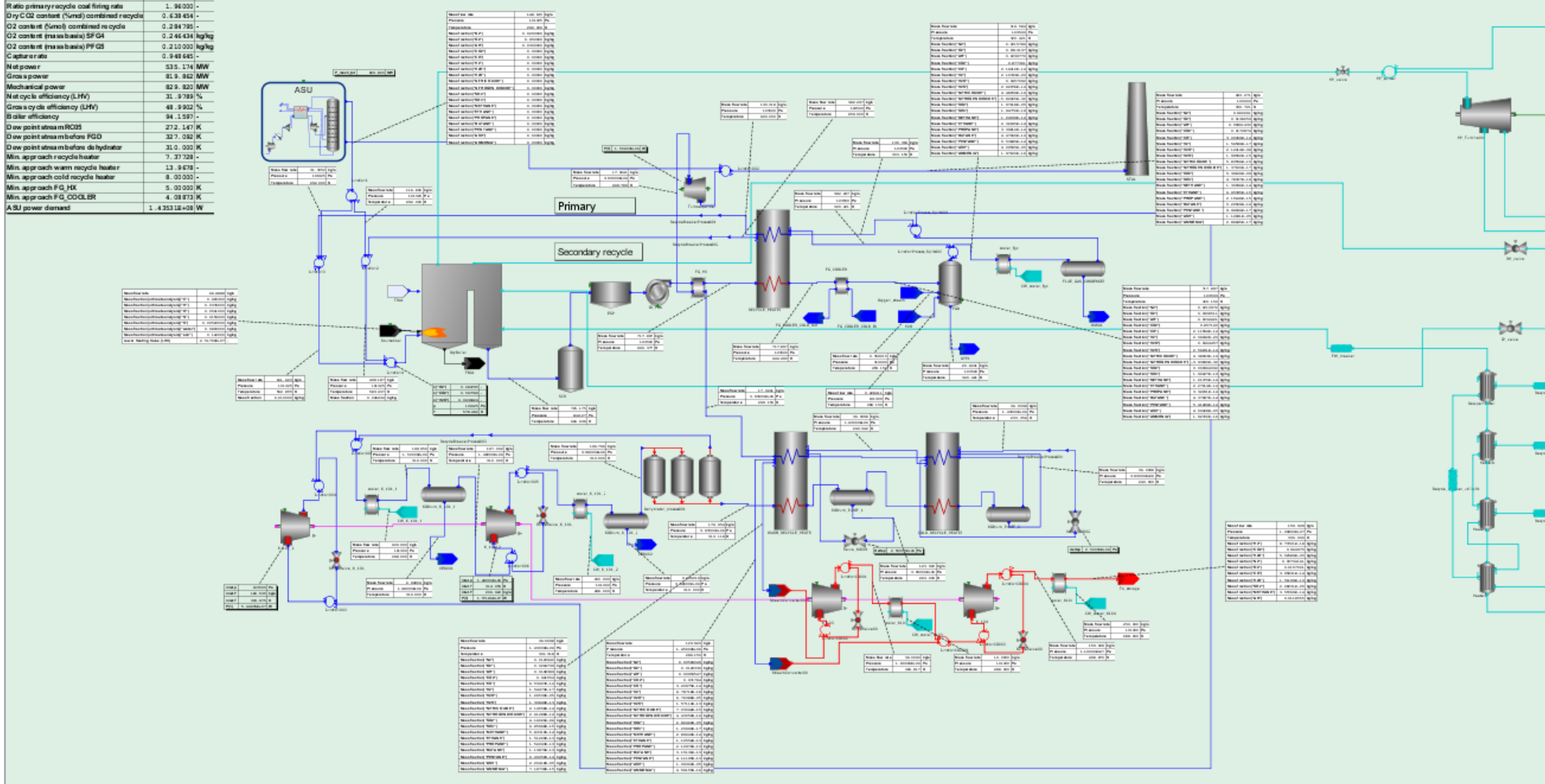
gCCS Power Plant library – conventional power generation CCGT power plant

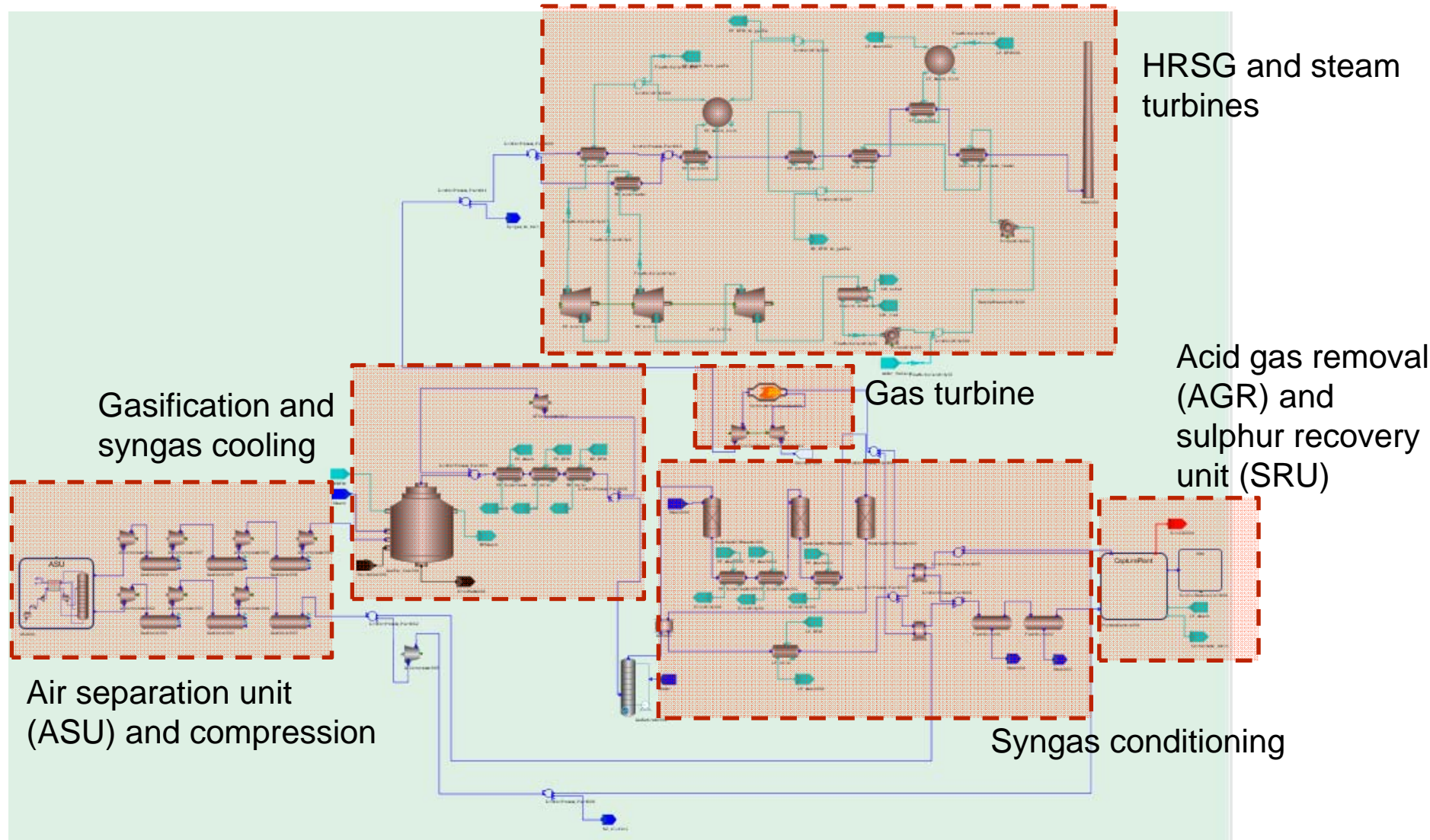


Oxyfuel system

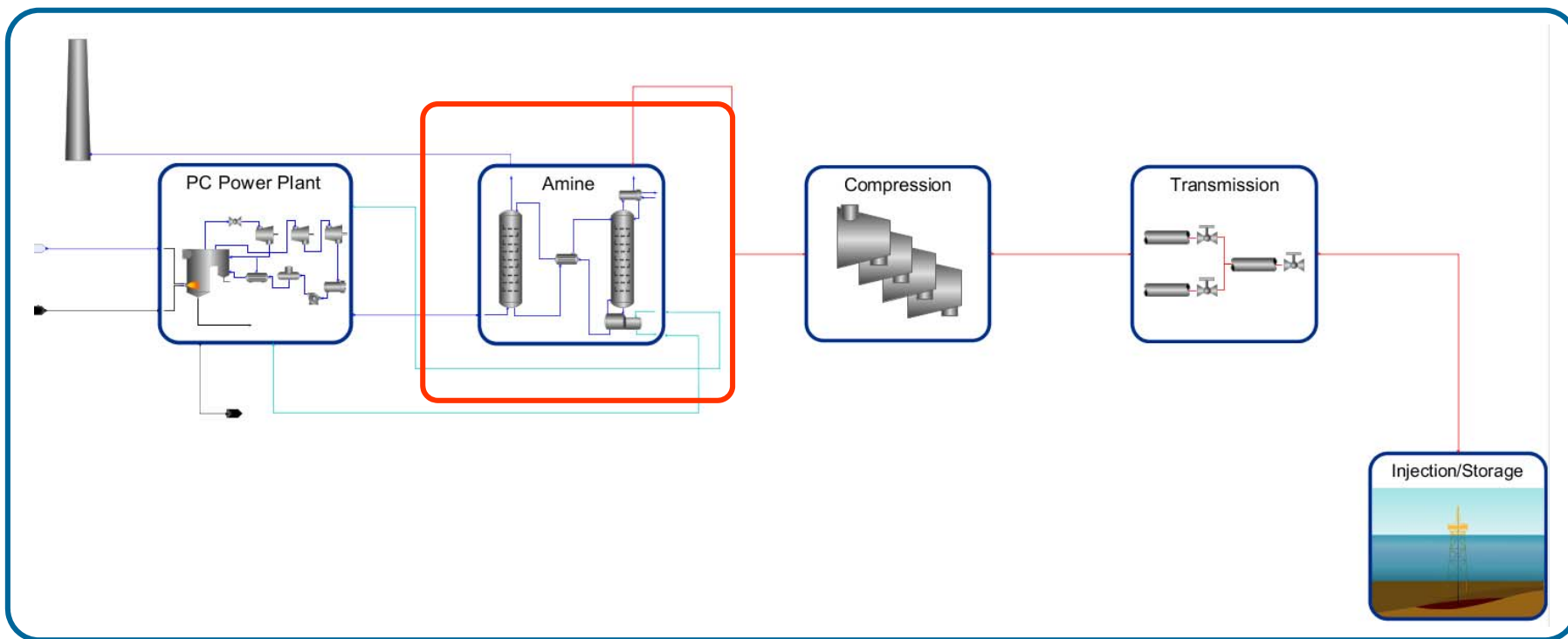


Total recycle ratio	0.740303	-
Ratio primary recycle coal firing rate	1.96303	-
Dry CO ₂ content (Nm ³) combined recycle	0.631454	-
O ₂ content (Nm ³) combined recycle	0.248793	-
O ₂ content (mass basis) SF G4	0.246434	kg/kg
O ₂ content (mass basis) SF G5	0.210303	kg/kg
Capex ratio	0.948443	-
Net power	535.174	MW
Gross power	819.962	MW
Mechanical power	829.820	MW
Net cycle efficiency (LHV)	31.9789	%
Gross cycle efficiency (LHV)	48.9902	%
Solar efficiency	34.1597	-
Dew point steam H2O5	273.147	K
Dew point steam before H2O2	327.326	K
Dew point steam before hydrator	310.003	K
Min. approach recycle heater	7.37328	-
Min. approach warm recycle heater	13.9478	-
Min. approach cold recycle heater	8.00303	-
Min. approach F.G. HX	15.00303	K
Min. approach F.G. COOLBR	4.08873	K
ASU power demand	1.43312+03	W



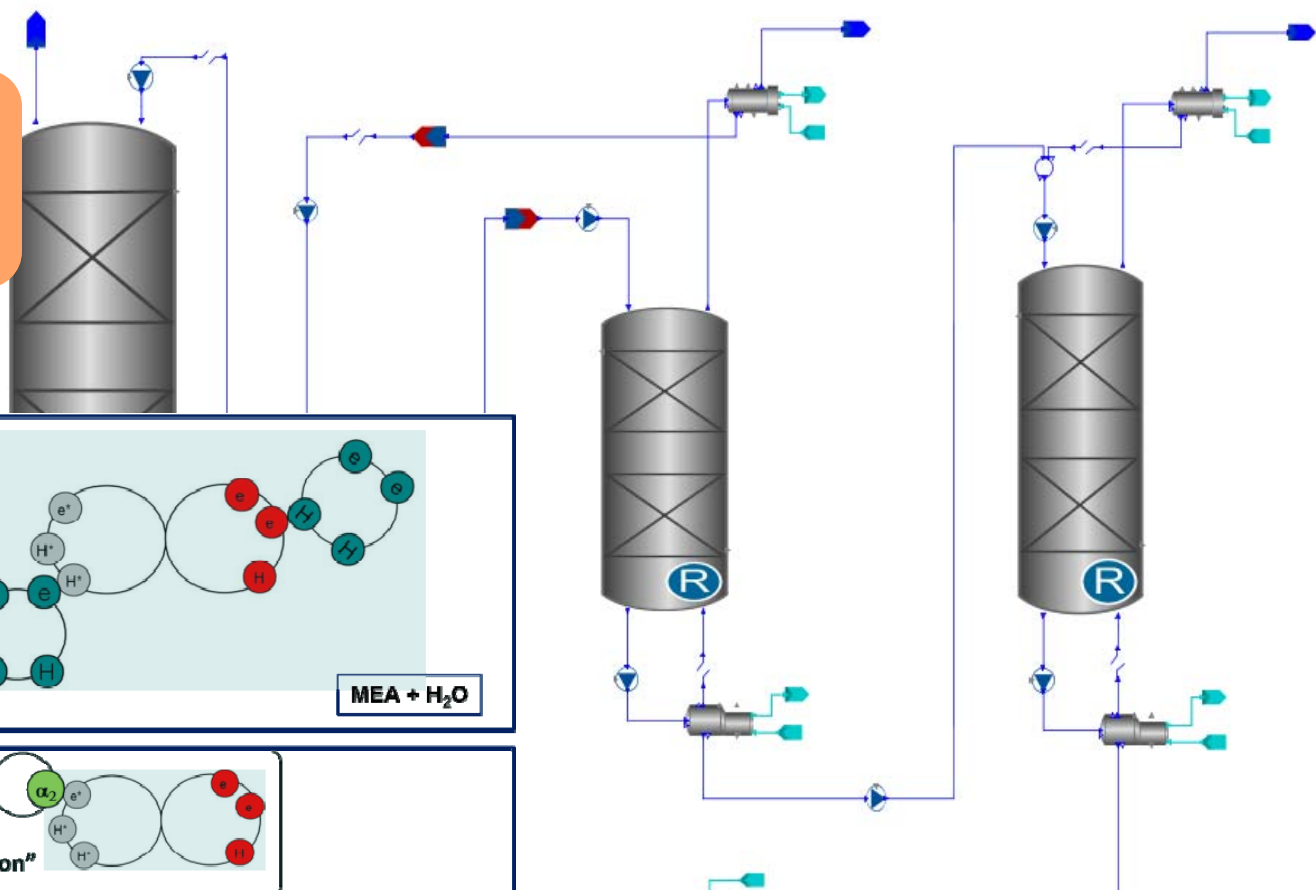
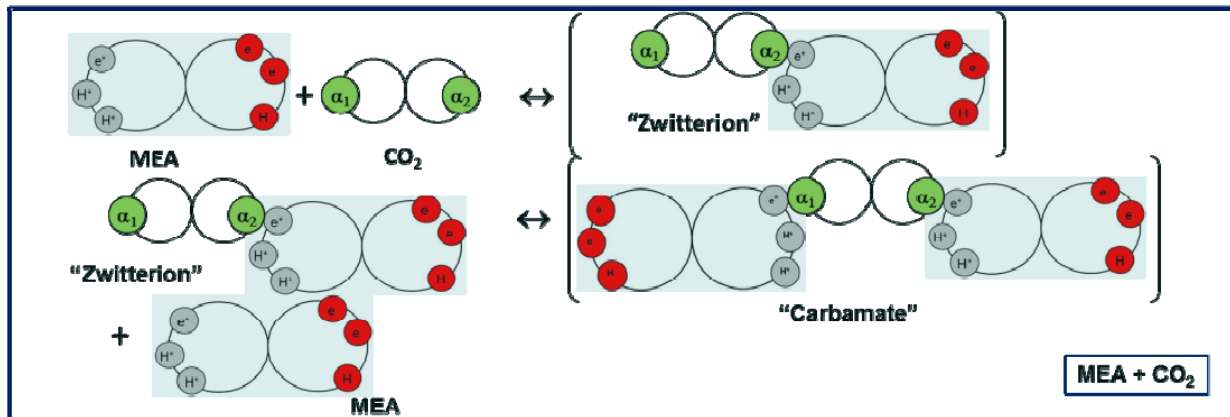
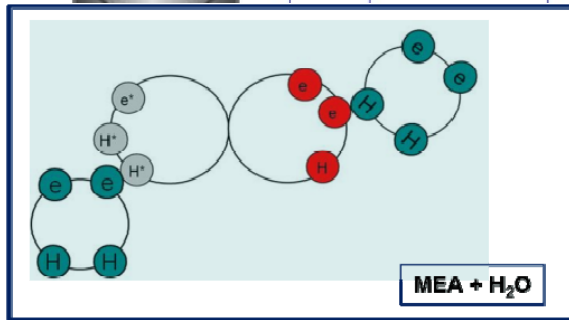
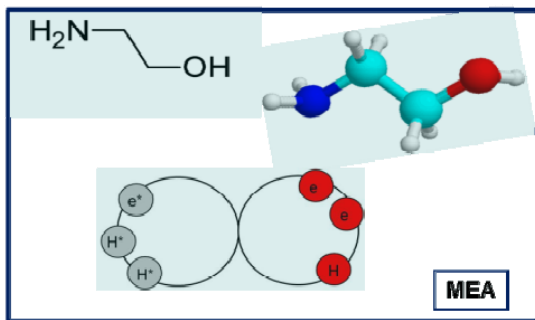


CO₂ Capture



Process and material models

gCCS process models

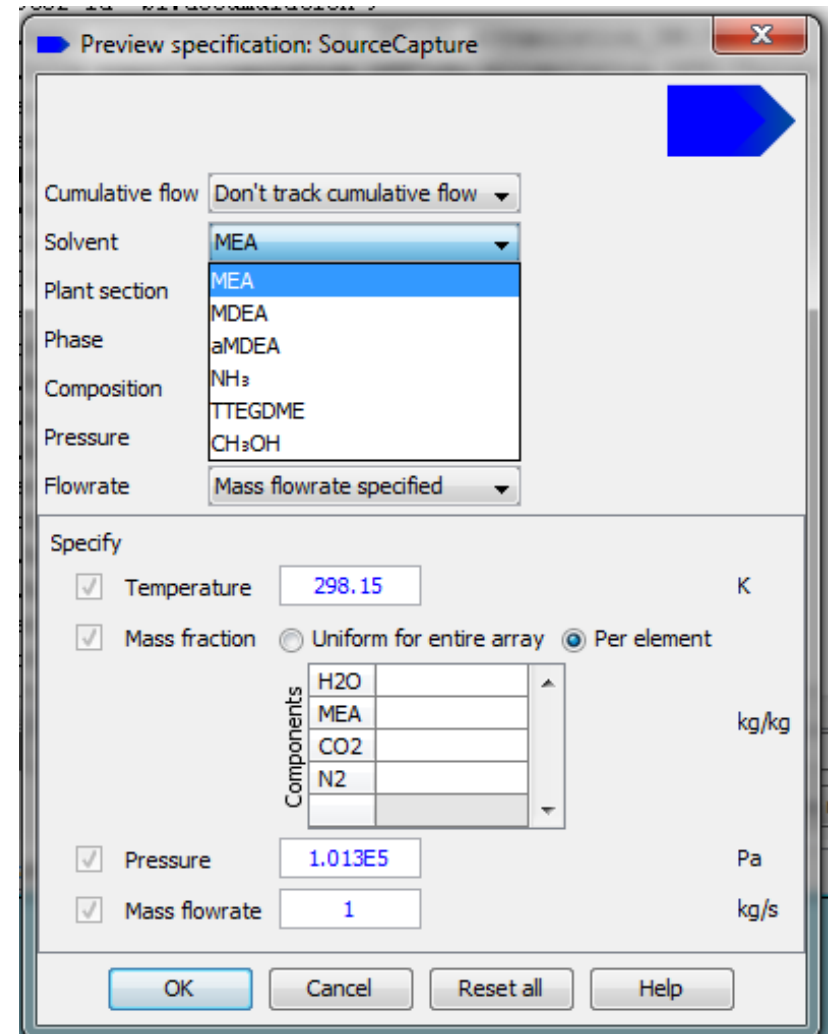


gSAFT material models

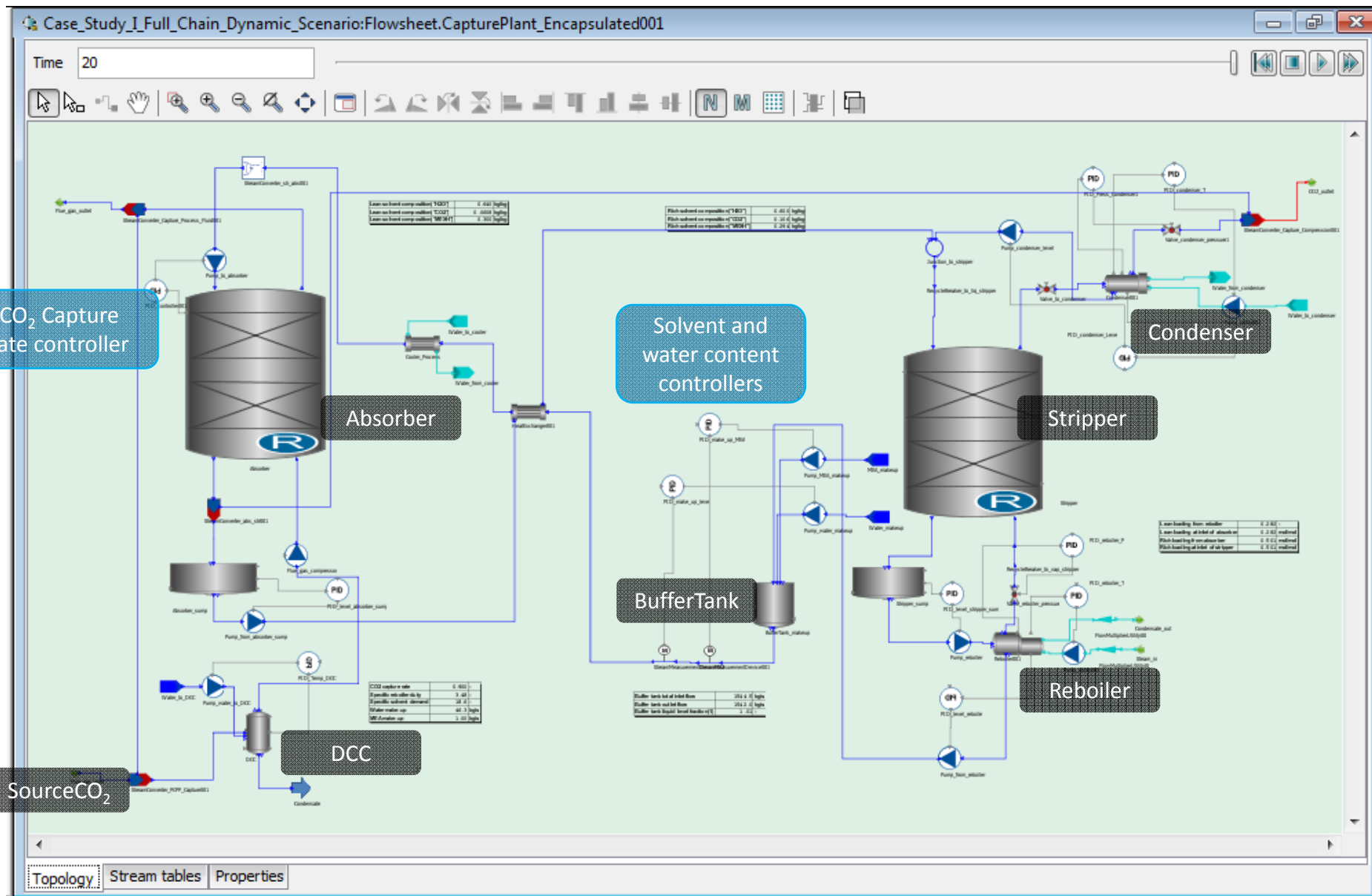
Current status



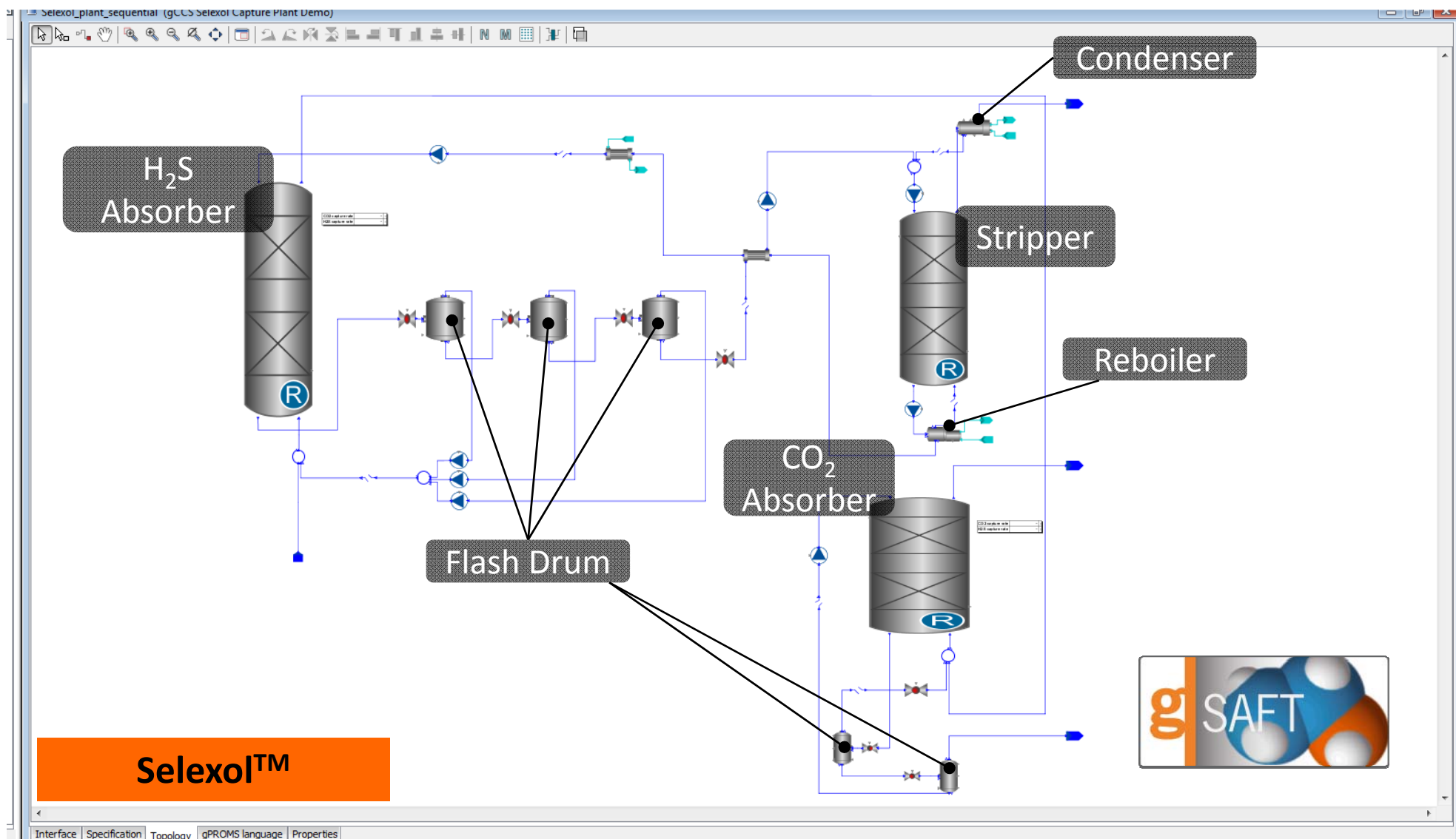
- Chemical absorption
 - MEA, MDEA activated with piperazine, NH₃
- Physical absorption
 - Mixtures of PEGDME (as those employed in the Selexol™ process) and methanol (Rectisol™ process)

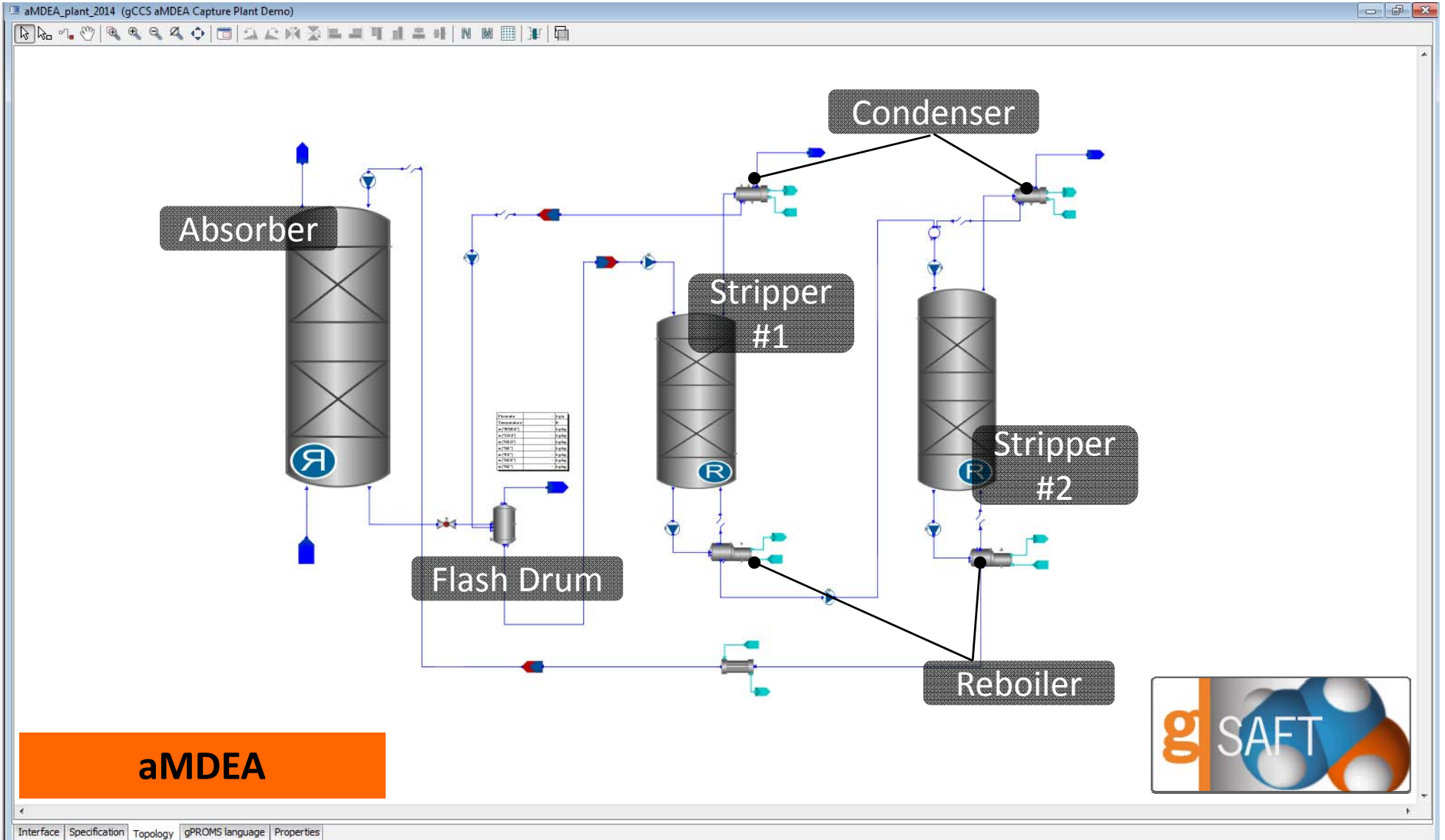


Chemical Absorption

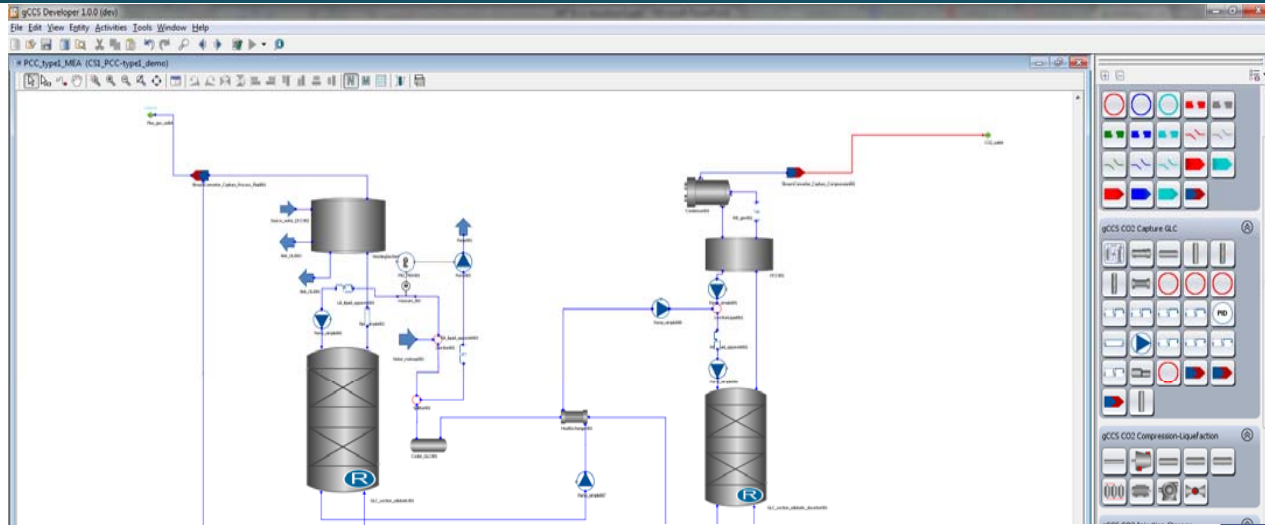


gCCS CO₂ Capture Library Physical absorption capture plant model





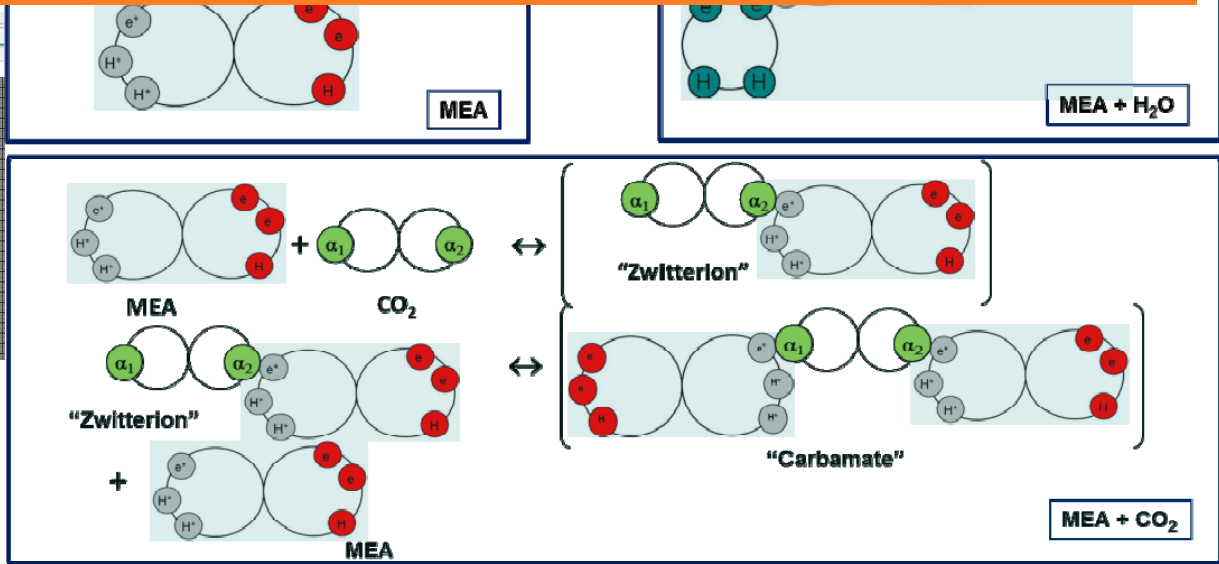
Solvent-based CO₂ capture optimisation



- Process design
- Configuration
- Equipment size
- Heat integration
- ...
- Process operation
- Solvent loading
- Flowrates
- Pressures, temperatures
- ...

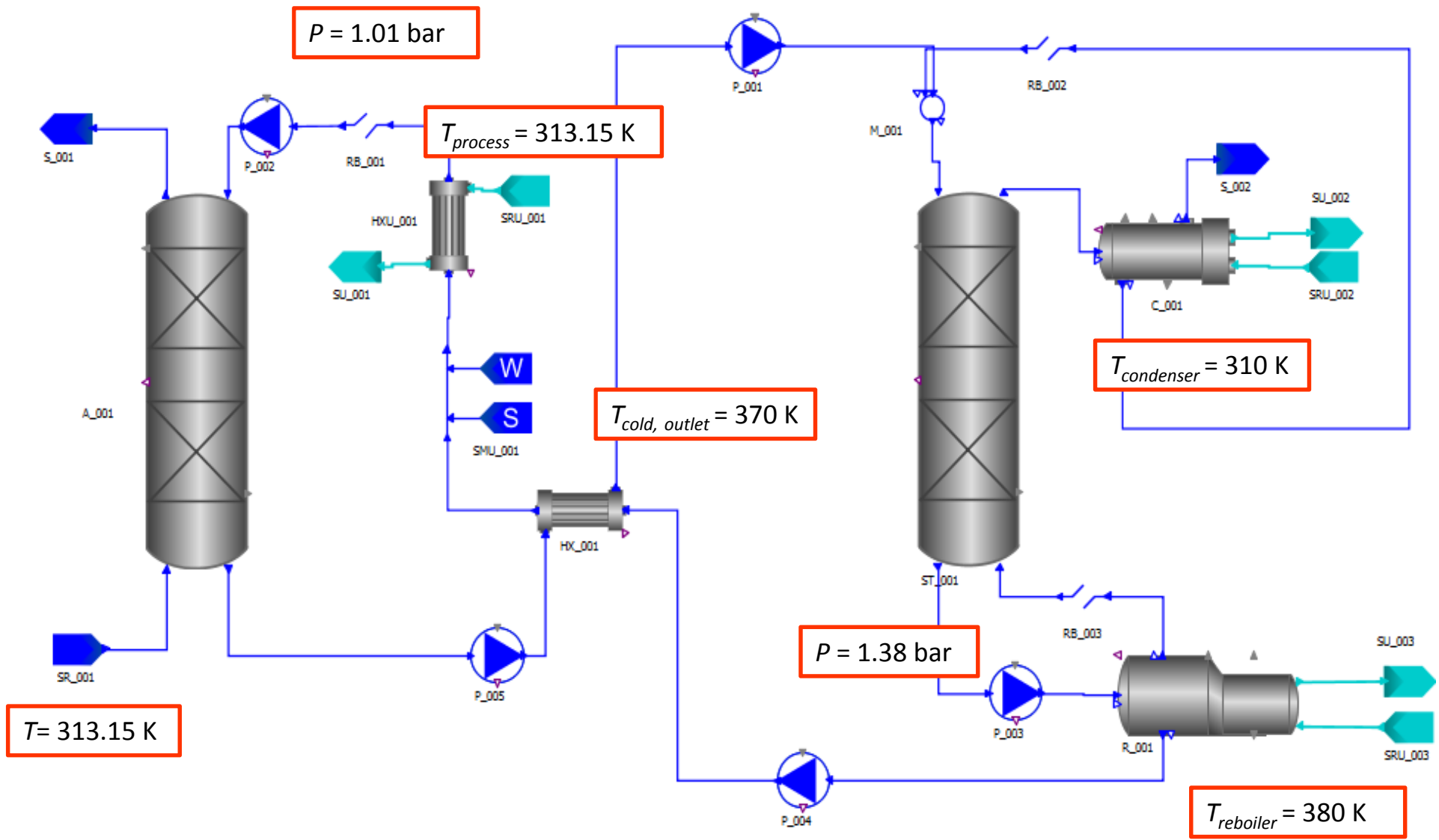
gCCS allows for all aspects to be optimised simultaneously achieving more economical solutions

Solvent design/ development
 Screening of candidates
 New molecules (group contribution method)
 New mixtures



Optimization example

Simple absorber and simple stripper configuration



Optimization example

Simple absorber and simple stripper configuration



- Objective function: reboiler heat duty
- Constraint: CO₂ capture > 90 %

Time Invariant Controls



	Final Value	Initial Guess	Lower Bound		Upper Bound	
			Value	Lagrange Multiplier	Value	Lagrange Multiplier
Flowsheet.P_003.Outlet.p	2.2850×10^5	1.3800×10^5	1.2550×10^5	0.0000	5.0000×10^5	0.0000
Flowsheet.R_001.T	3.9778×10^2	3.8000×10^2	3.7000×10^2	0.0000	4.2300×10^2	0.0000
Flowsheet.SMU_001.Src_F	5.4882×10^{-1}	1.0000	2.0000×10^{-1}	0.0000	1.6000	0.0000
Flowsheet.SMU_001.w_solvent("PZ")	4.0000×10^{-1}	3.6400×10^{-1}	3.6400×10^{-1}	0.0000	4.0000×10^{-1} *	5.3383×10^{-2}

* indicates an active bound

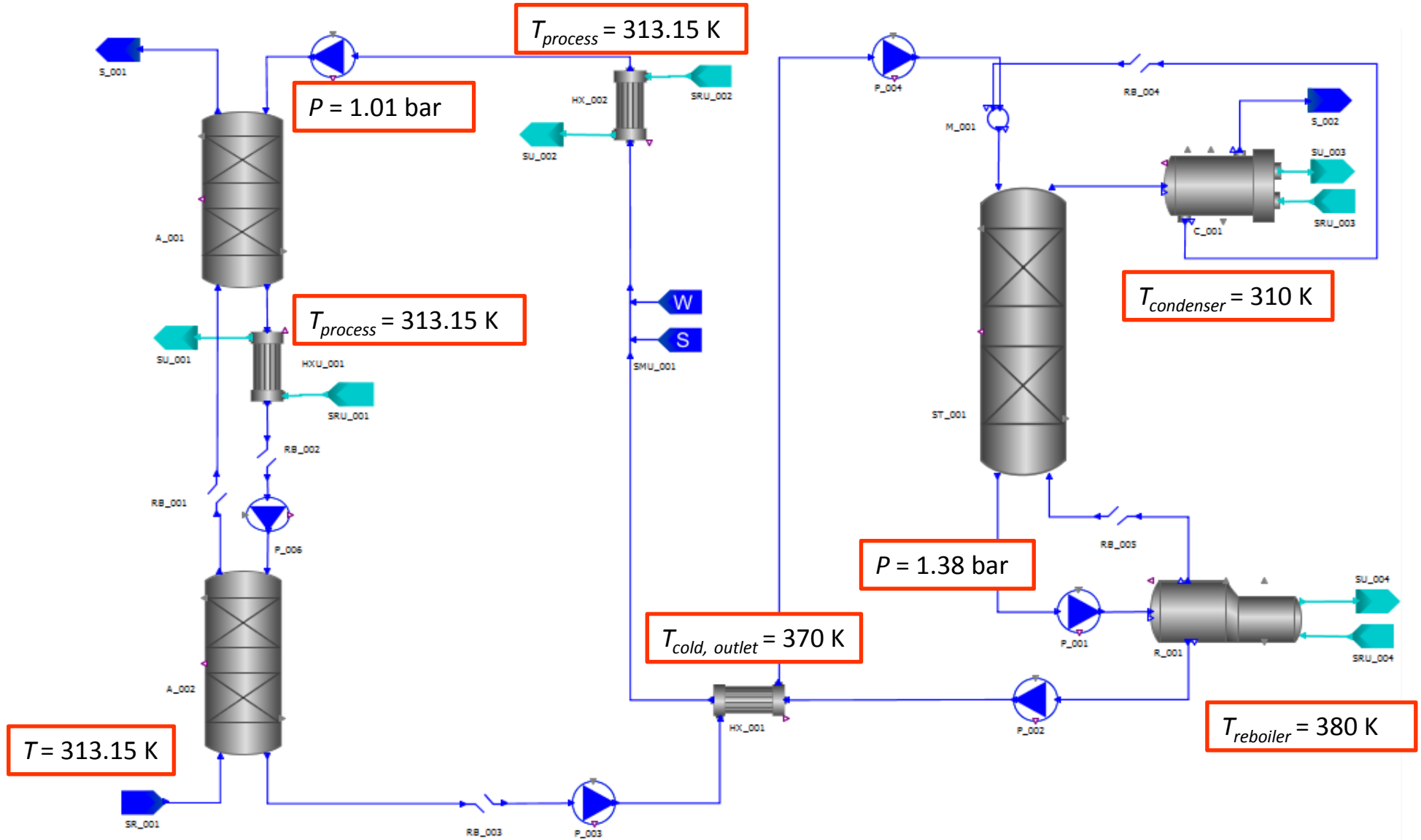
Variable	Initial value	Lower bound	Upper bound	Optimisation value
CO ₂ capture (%)	88.8	90.0	100	90.5
(kJ/kg CO ₂)	5229	-	-	4230

- 11 %

85

Optimization example

Intercooled absorber and simple stripper configuration



Optimization example

Intercooled absorber and simple stripper configuration



- Objective function: reboiler heat duty
- Constraint: CO₂ capture > 90 %

Time Invariant Controls



	Final Value	Initial Guess	Lower Bound		Upper Bound	
			Value	Lagrange Multiplier	Value	Lagrange Multiplier
Flowsheet.HXU_001.T_out_process	2.9815×10^2	3.1315×10^2	2.9815×10^2 *	2.4783×10^{-4}	3.1415×10^2	0.0000
Flowsheet.P_001.Outlet.p	1.5175×10^5	1.3800×10^5	1.2500×10^5	0.0000	5.0000×10^5	0.0000
Flowsheet.R_001.T	3.7583×10^2	3.7665×10^2	3.7000×10^2	0.0000	4.2315×10^2	0.0000
Flowsheet.SMU_001.Src_F	9.4647×10^{-1}	1.0000	2.0000×10^{-1}	0.0000	2.0000	0.0000
Flowsheet.SMU_001.w_solvent("PZ")	4.0000×10^{-1}	3.6400×10^{-1}	3.5000×10^{-1}	0.0000	4.0000×10^{-1} *	2.0898×10^{-2}

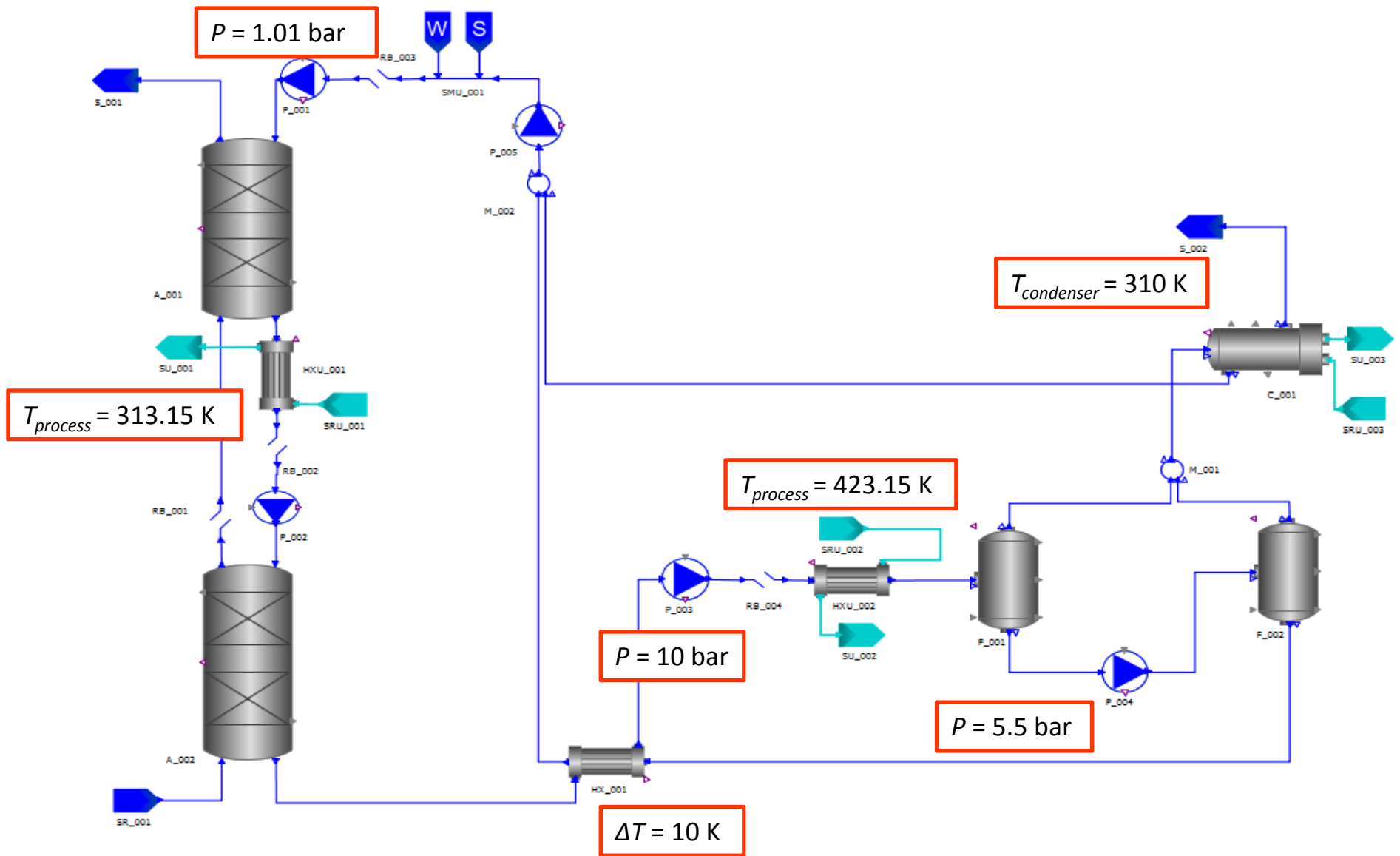
* indicates an active bound

Variable	Initial value	Lower bound	Upper bound	Optimised value
CO ₂ capture (%)	98.6	90.0	100	90.4
(kJ/kg CO ₂)	4924	-	-	4239

- 13 %

87

Optimization Example: Intercooled absorber with two flashes



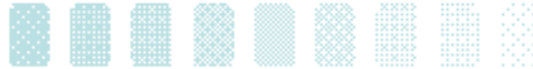
Optimization Example:

Intercooled absorber with two flashes



- Objective function: CO₂ capture

Time Invariant Controls



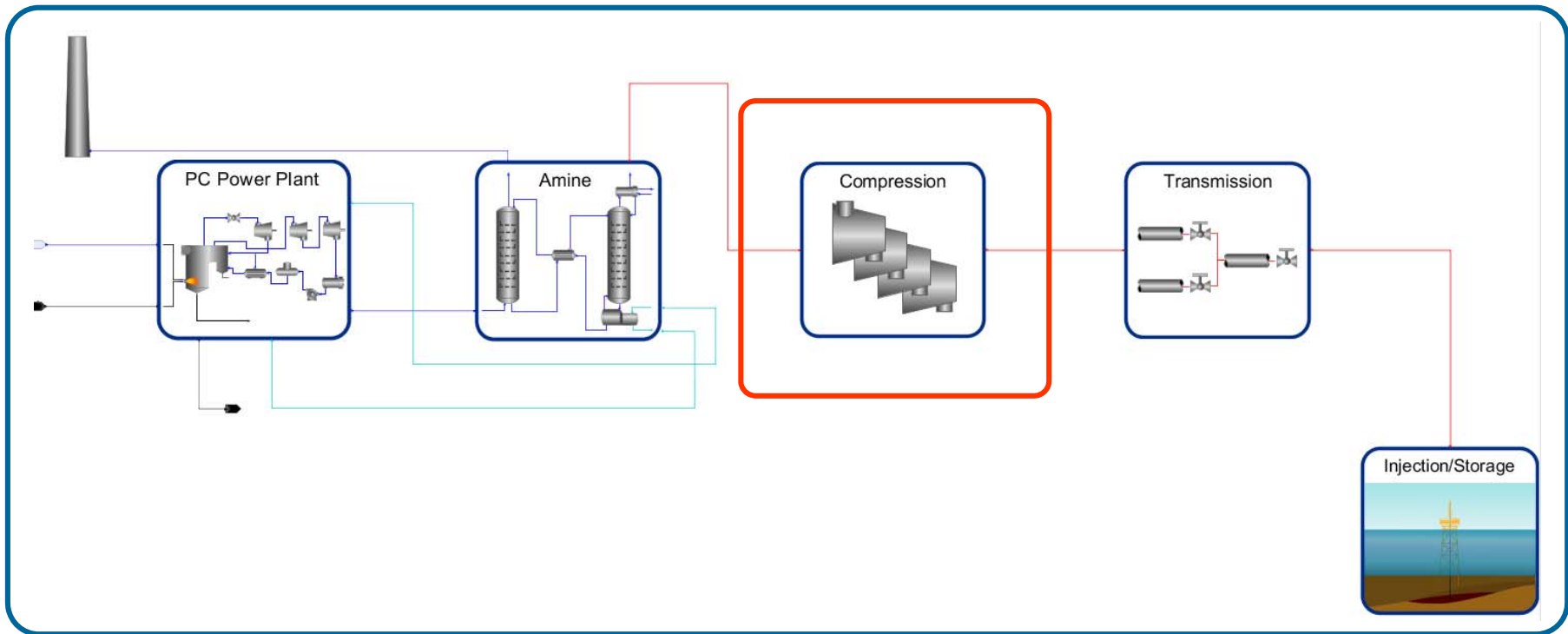
	Final Value	Initial Guess	Lower Bound		Upper Bound	
			Value	Lagrange Multiplier	Value	Lagrange Multiplier
Flowsheet.HXU_001.T_out_process	3.0703×10^2	3.1315×10^2	2.9815×10^2	0.0000	3.1400×10^2	0.0000
Flowsheet.P_003.Outlet.p	8.1893×10^5	1.0000×10^6	5.0000×10^5	0.0000	1.2000×10^6	0.0000
Flowsheet.P_004.Outlet.p	4.7729×10^5	5.5000×10^5	2.0000×10^5	0.0000	1.0000×10^6	0.0000
Flowsheet.SMU_001.Src_F	1.0403	1.0000	4.0000×10^{-1}	0.0000	1.6000	0.0000



Variable	Initial value	Lower bound	Upper bound	Optimised value
CO ₂ capture (%)	63.2	-	-	77.0
(kJ/kg CO ₂)	4372	-	-	4119

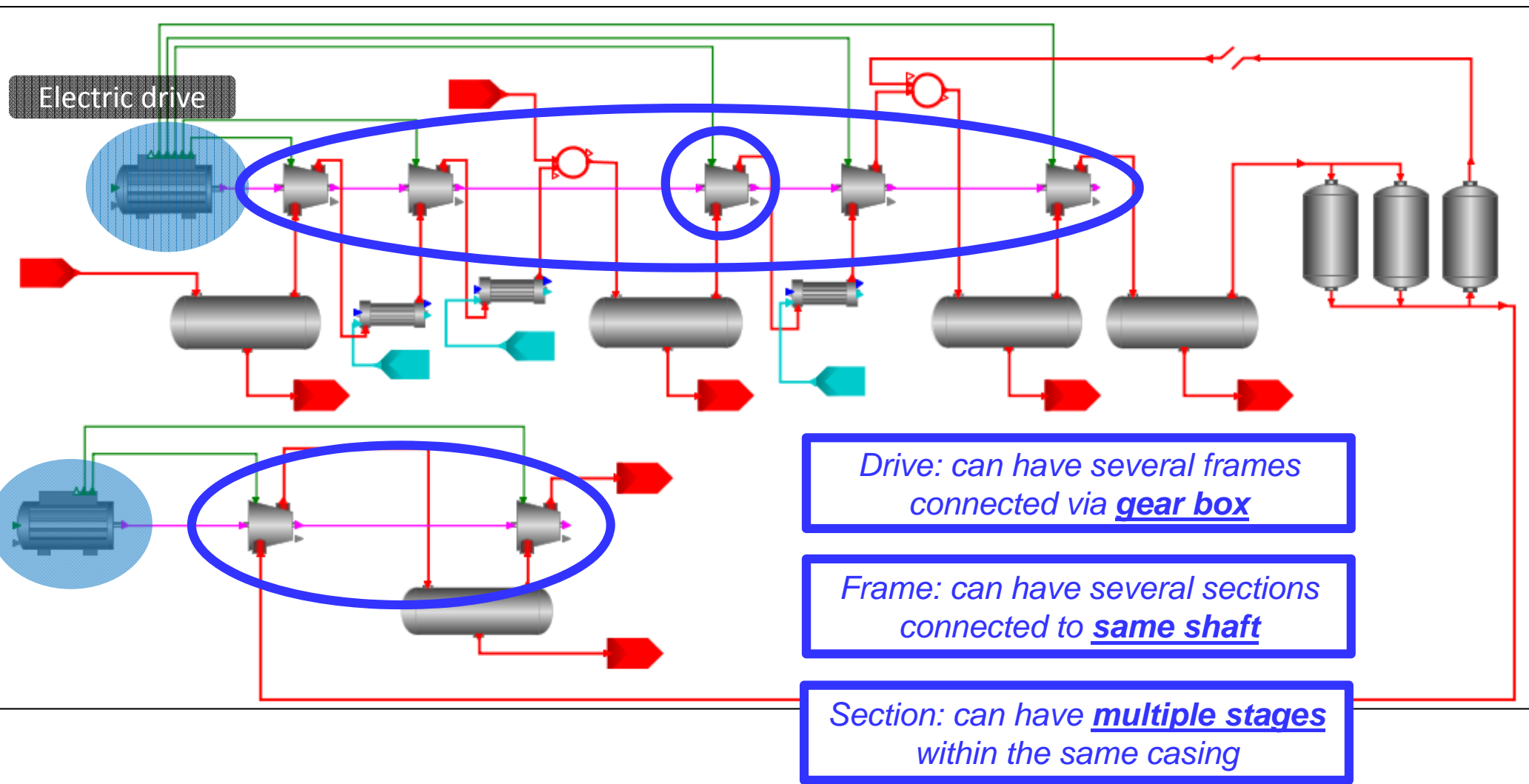
+ 22%
- 6%

Compression

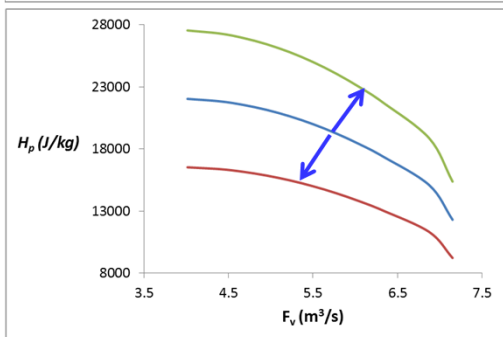
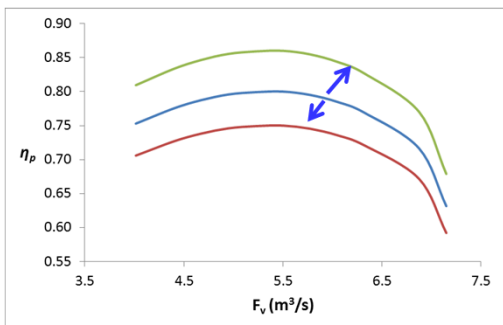


Multi-section compressor train

Basic concepts



Compressor model – performance maps



```

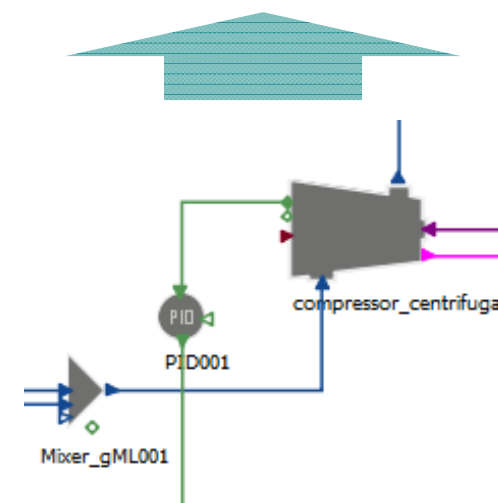
],
  "Diameter" : 1.066864516,
  "DesignSpeed" : 69.95,
  "Map" :
  [
    {
      "Curve" :
      [
        [0.10847, 2.387901, 0.850614],
        [0.112603, 2.373763, 0.860395],
        [0.116736, 2.351798, 0.868467],
        [0.120868, 2.321925, 0.874854],
        [0.125001, 2.282775, 0.879213],
        [0.129134, 2.230553, 0.880363],
        [0.133266, 2.164399, 0.877854],
        [0.137399, 2.085194, 0.87204 ],
        [0.141531, 1.986933, 0.860782],
        [0.145664, 1.84251, 0.834881],
        [0.149797, 1.610725, 0.778101]
      ]
    }
  ]

```

Specify

Compressor map specification: 1-D dimensionless (Phi(Theta) and eta(Theta))

Performance map: MapC.json



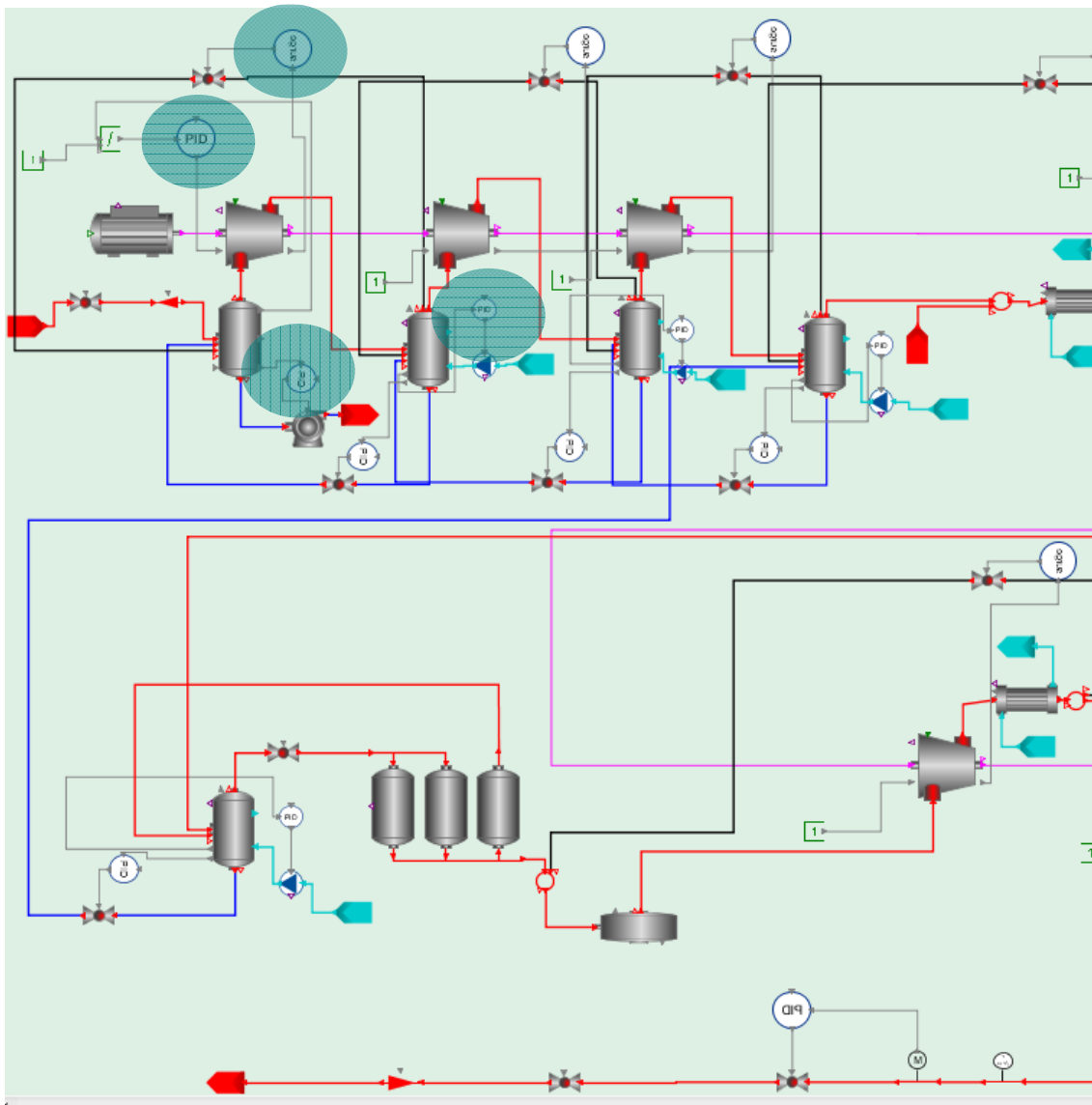
Performance map data (flow/head and flow/eff)

Converted to txt file format in ProcessBuilder (including multiple stages)

Compressor model reads performance map file

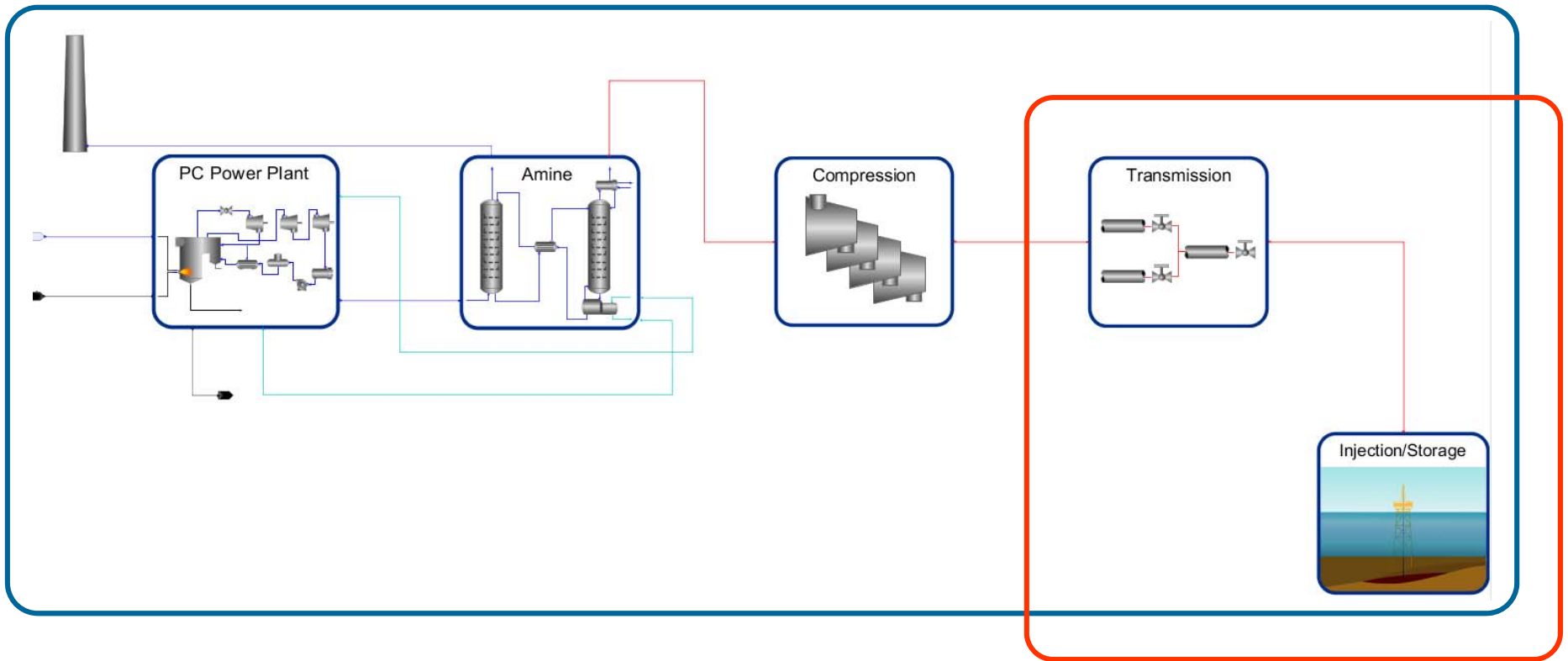
Multi-section compressor train

Control system - Demo

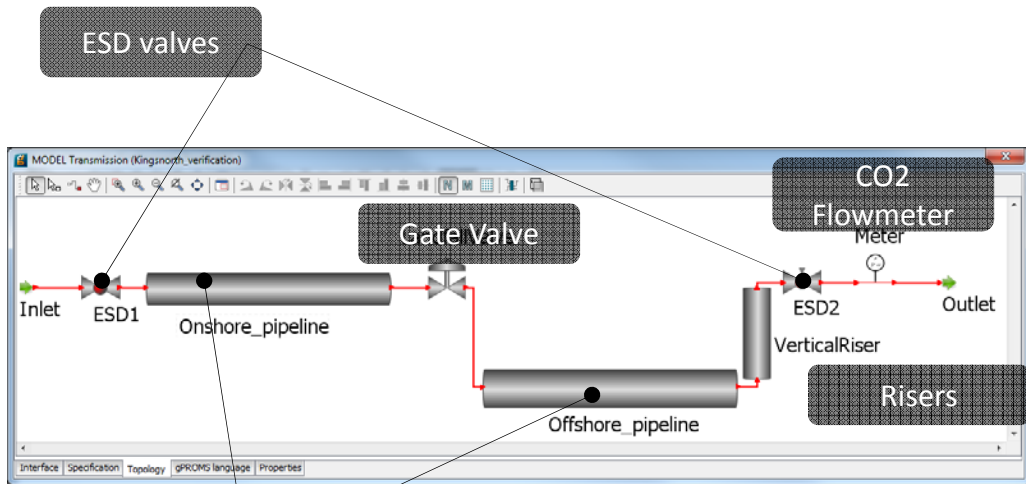


- Dynamics accounted for
 - KO-Drum mass/energy holdup
 - Shaft and compressor inertia
 - Valve dynamics
 - Opening time
 - Closing time
 - Controller parameters
- Suction pressure
 - IGV control
 - VFD control
- For every compression stage
 - Anti-surge control
 - Discharge temperature control
 - KO-Drum level control
- All safety valves
 - ESD valve
 - Check valve

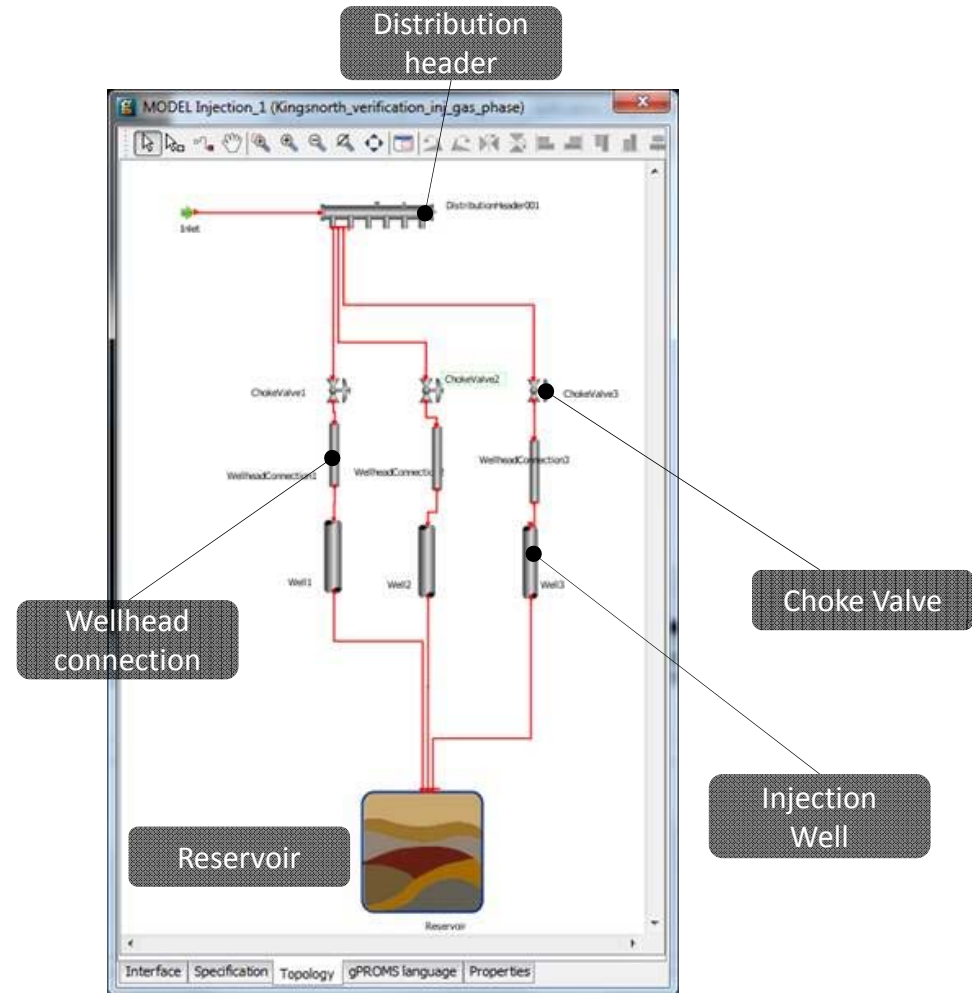
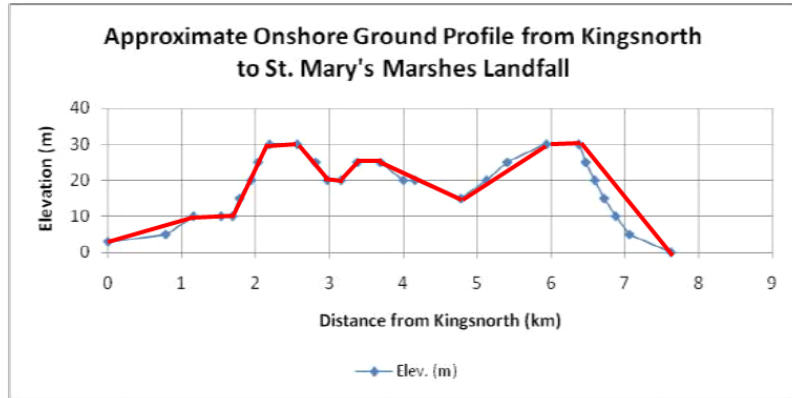
Transmission & injection



Transmission and Injection



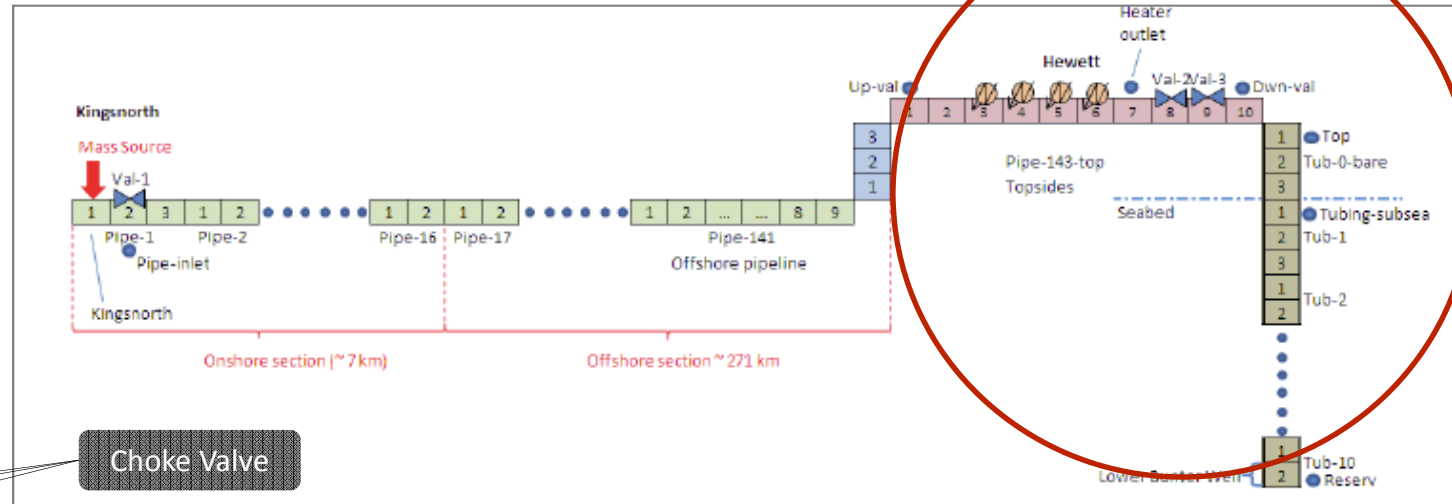
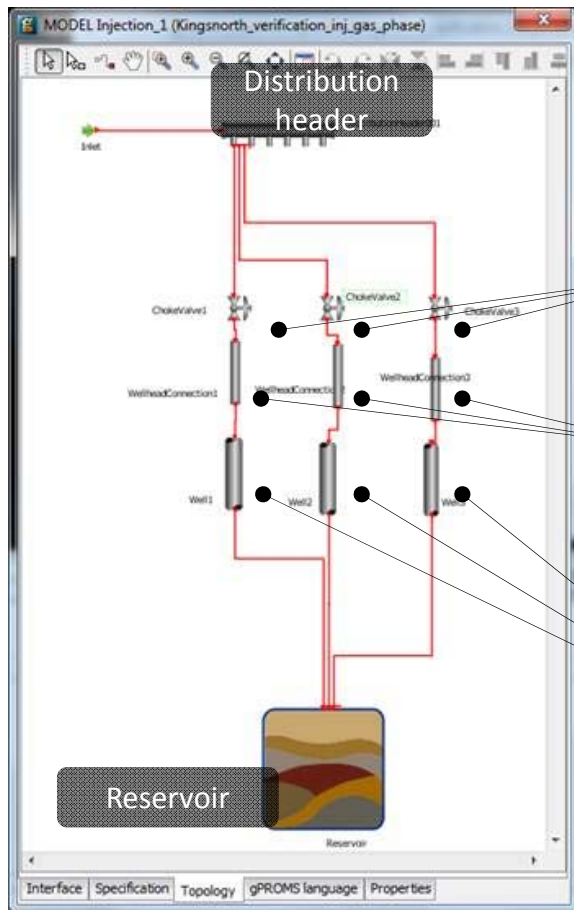
Pipelines – including topography



Transmission and Injection



Model verification: e.g.
Kingsnorth FEED -
Injection/storage

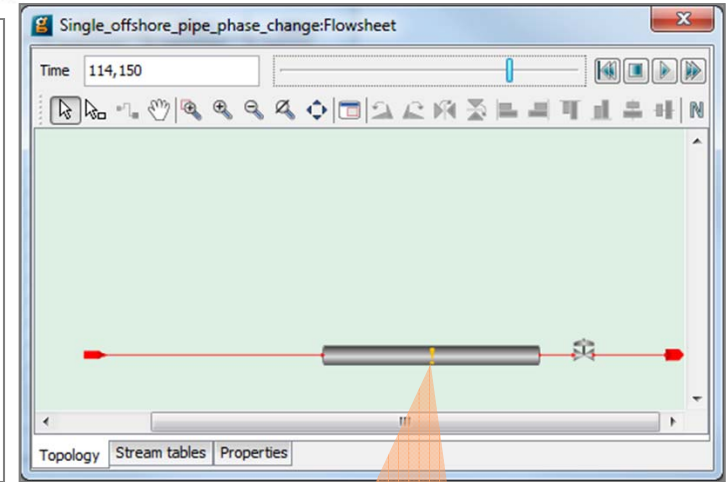
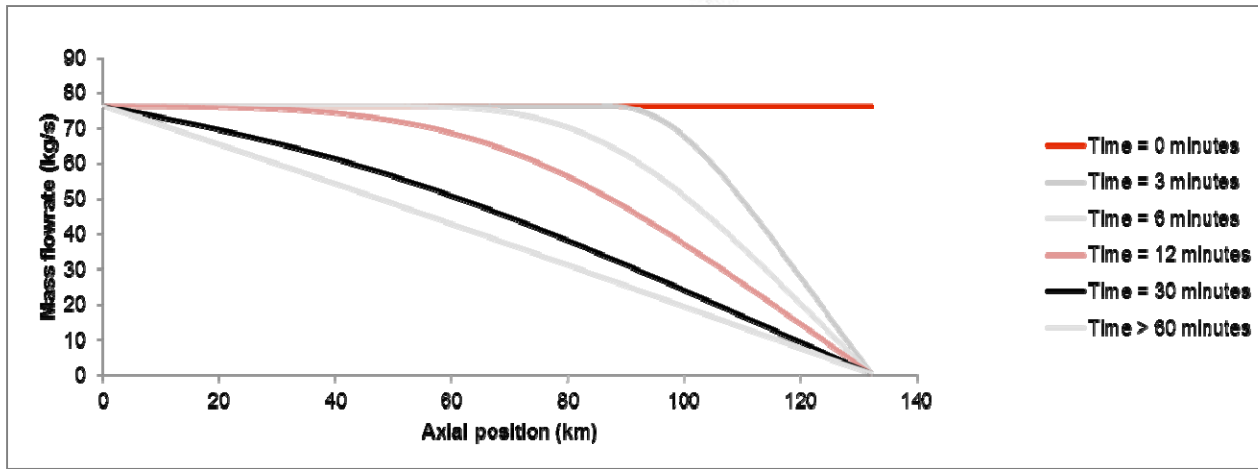


For gas phase operation (reservoir pressure 2.1 barg)	Kingsnorth	gCCS	% Error (abs K for temps)
ΔP between Reservoir and Bottomhole (bar)	5.4	5.36	~0.6
ΔP between Bottomhole and downstream the choke valve (bar)	13.3	13.3	~0
Fluid temperature at Bottomhole (K)	279.05	280.9	-1.85

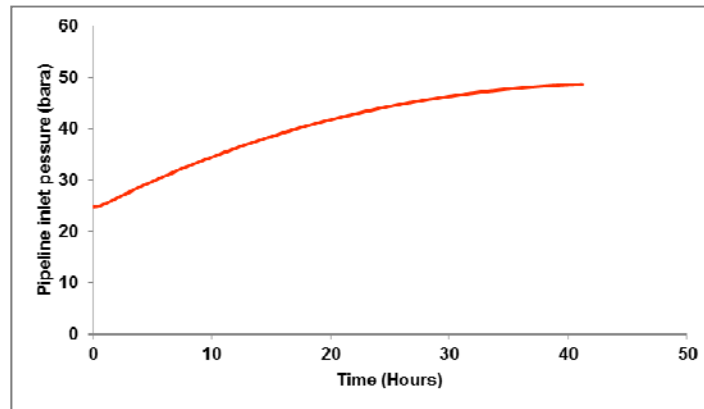
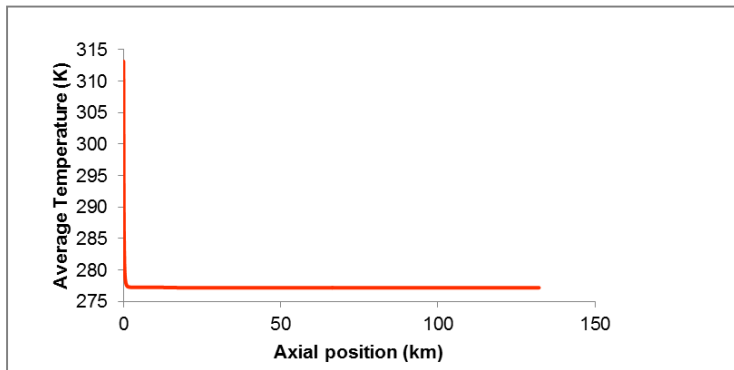
Example – line packing



■ System dynamics following downstream valve closure



Warning: Phase change identified!



Applications of gCCS: Case Studies

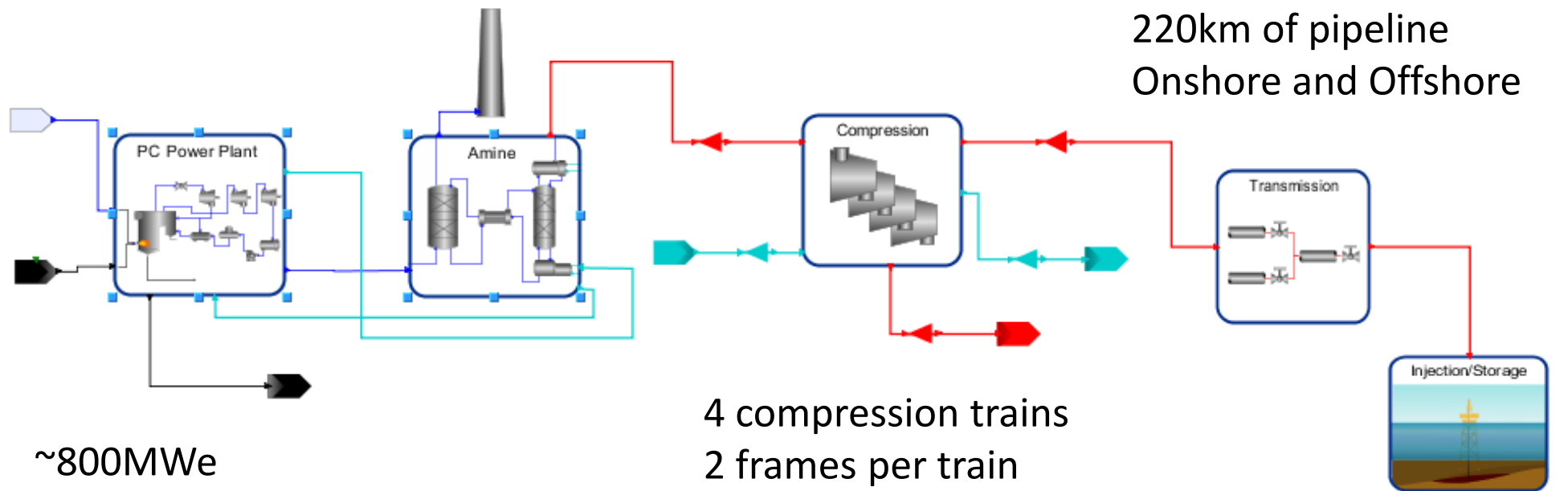


1. Process integration in CCS chains and networks

CCS Chain model developed in gCCS



Chemical absorption
MEA solvent
90% CO₂ capture



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

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

220km of pipeline
Onshore and Offshore

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

Steady-state scenarios



Scenario	Description	Power plant operation (% of nominal load)	Capture plant operation (CO2 % captured)
SS1.1 (a,b,c)	Base Load Power Plant	(a) 100%; (b) 75%; (c) 50%	0% (no capture)
SS1.2 (a, b)	Base load CCS Chain	100%	(a) 90%; (b) 50%
SS1.3 (a, b)	Part Load Analysis	(a) 75%; (b) 50%	90%
SS1.4	Extreme Weather: Max Summer	100%	90%
SS1.5	Extreme Weather: Min Winter	100%	90%

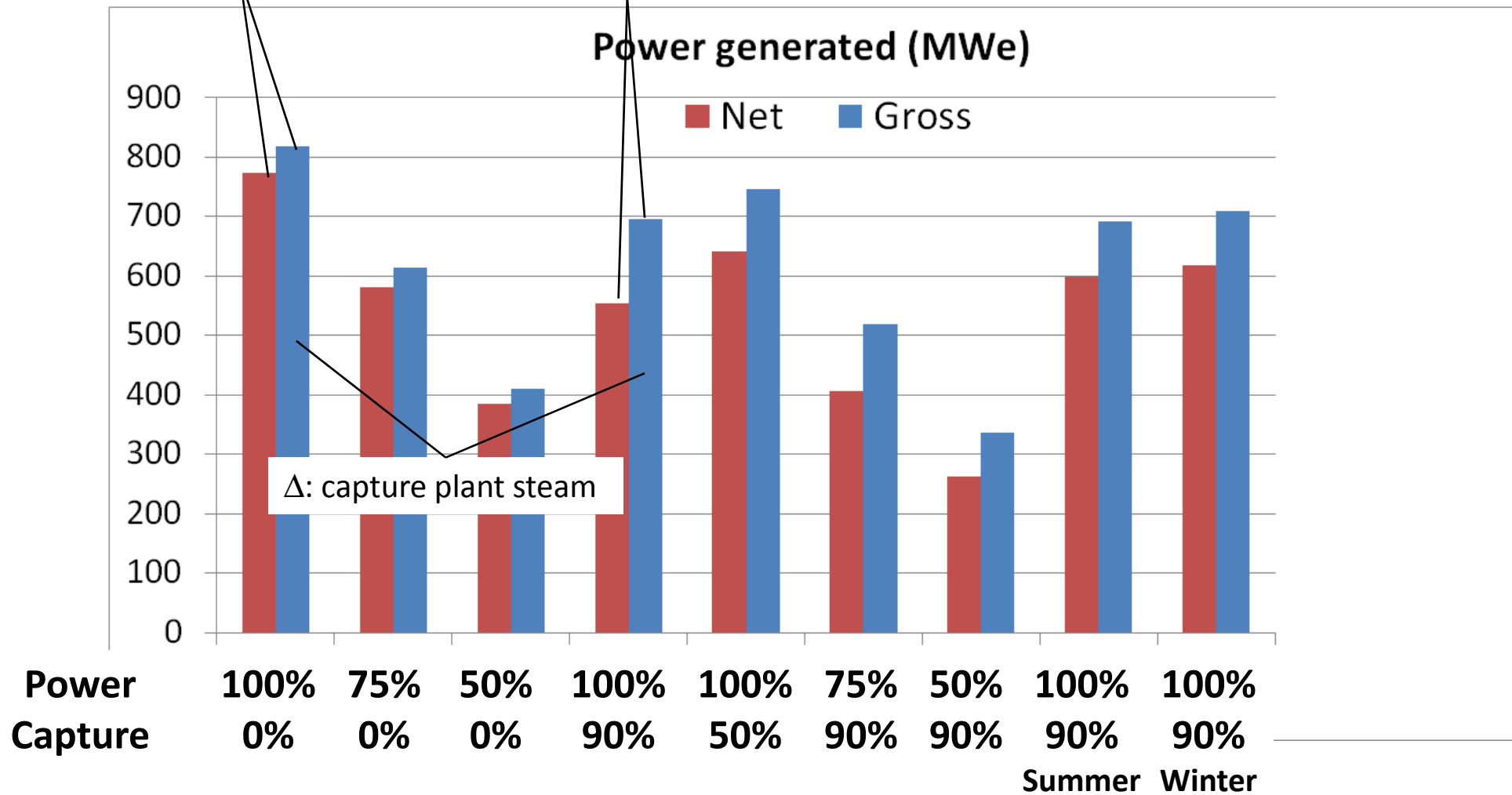
Temperatures (°C)	Affected sub-systems	Base Case	Extreme Summer	Extreme Winter
Cooling water	Power, Capture, Compression	18	22	7
Air	Power, Transmission, Injection	15	30	-15
Sea water	Transmission, Injection	9	14	4
NB. Geothermal gradient of +27.5°C / km				

Steady-state analysis

Power generation



Δ : coal milling
 + power plant auxiliaries
 Δ : coal milling
 + power plant auxiliaries
 + CO₂ compression



Applications of gCCS: Case Studies

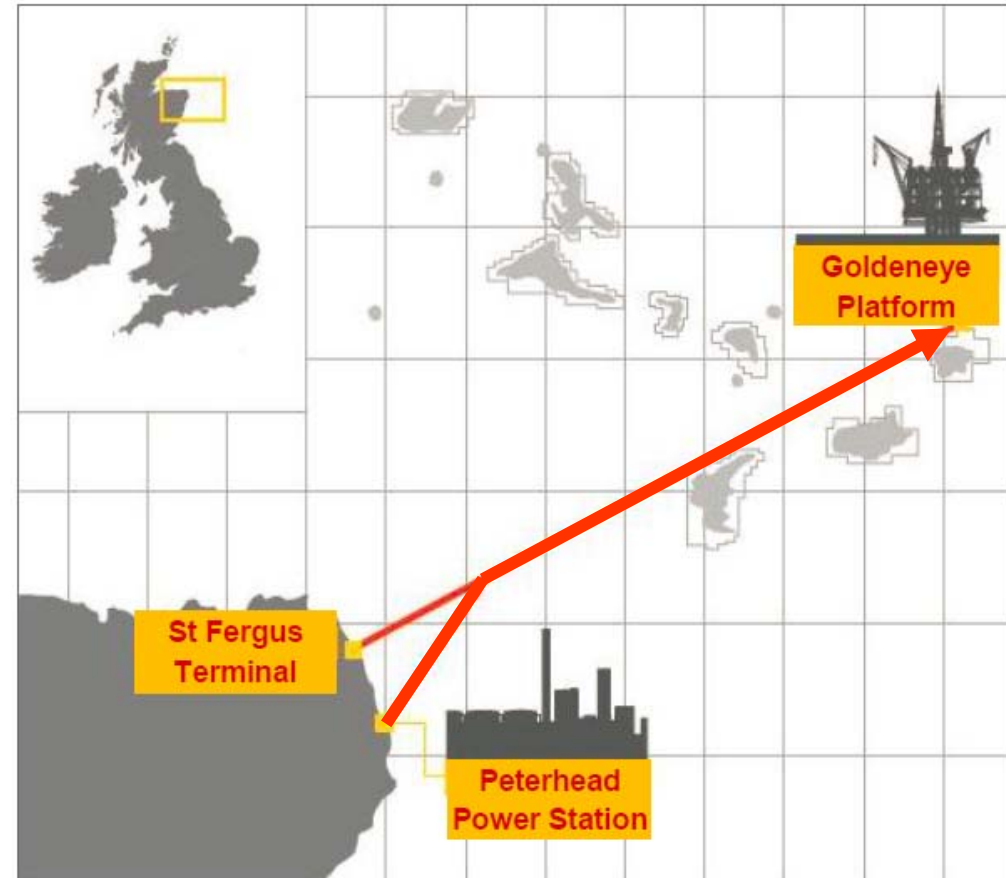


2. Shell Peterhead CCS project

The Shell Peterhead CCS project



- **World First** – first planned full-scale CCS project on a gas-fired power station
- **Where** – capture at Peterhead Power Station; storage in depleted Goldeneye gas reservoir (100 km off shore)
- **Technology** – post-combustion capture using amines.
- **Impact** – 10 to 15 million tonnes of CO₂ over a 10- to 15-year period (90% CO₂ capture from one turbine)



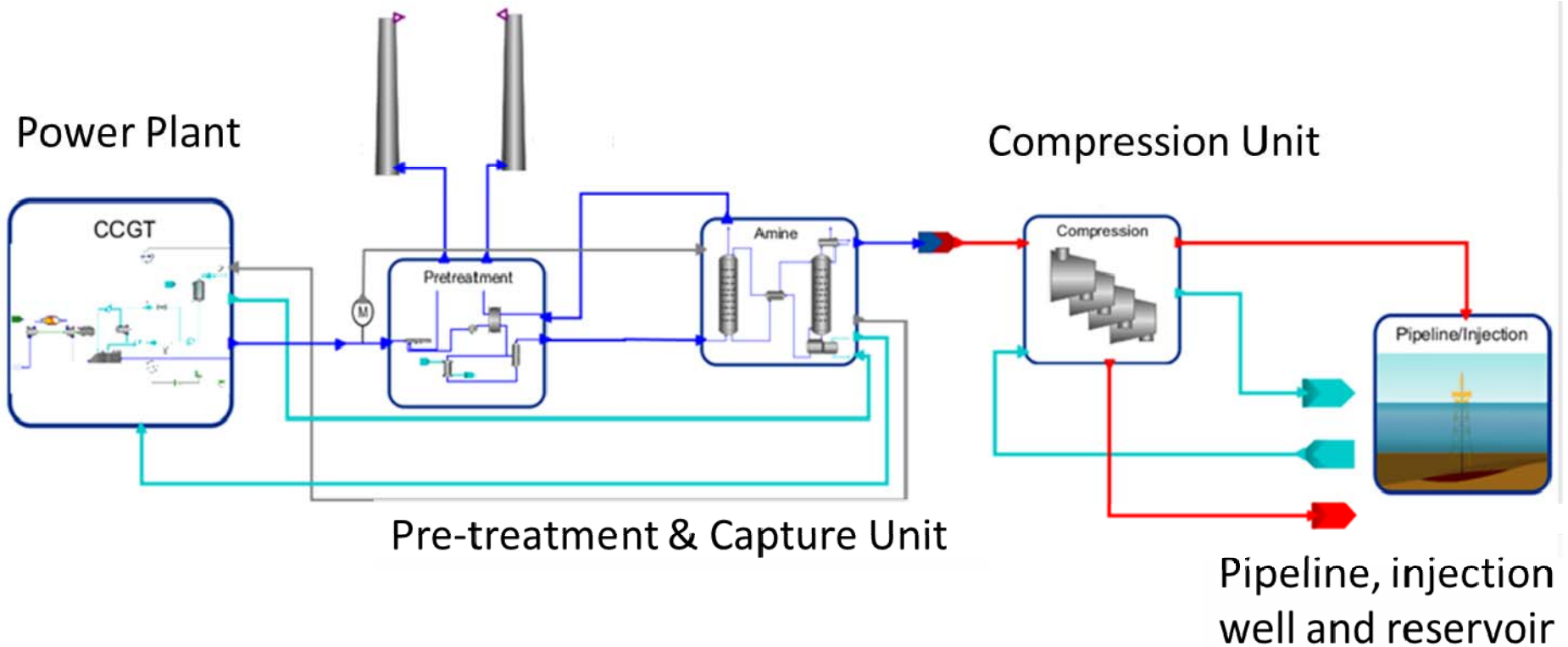
Modelling Project Objectives



- Develop full chain model from FEED deliverables
- High level verification of the overall CCS plant control philosophy
- Simulate dynamic operation scenarios including start-up, shut-down and various failure modes
- Analyse the simulation results to identify improvements to the existing operating procedures, which need to be followed up in detailed engineering studies.



Full chain flowsheet screenshot

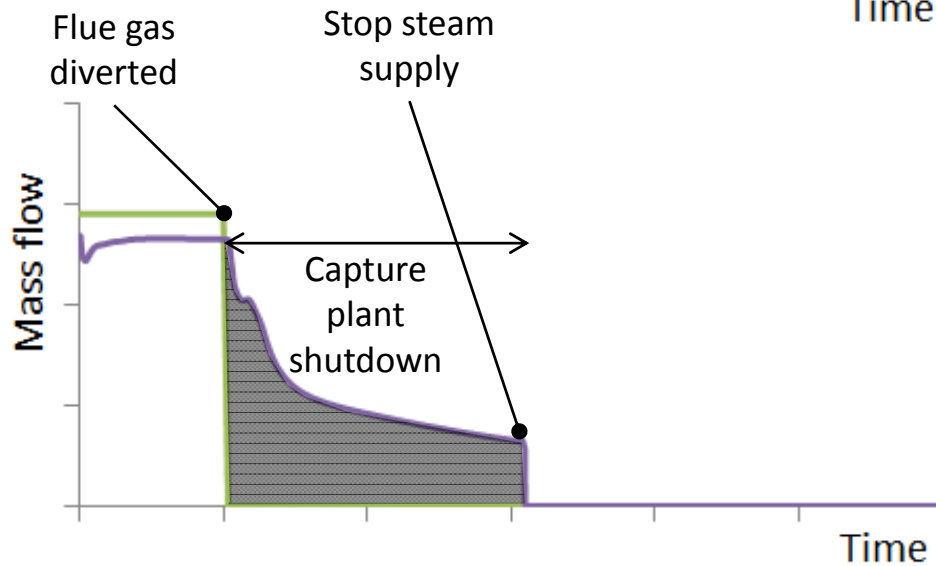
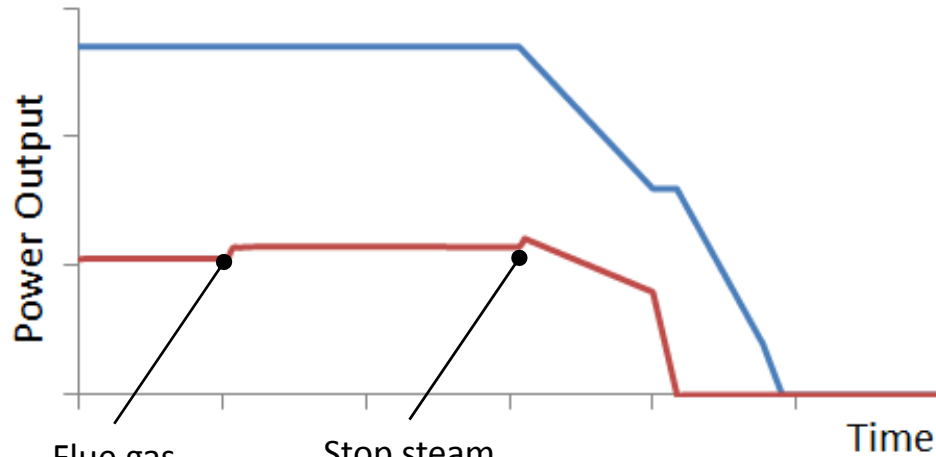


- 18,700 equations/variables
 - 17,800 algebraic
 - 900 differential
- Computation time (on laptop computer)
 - ~14h for whole CCS chain start-up

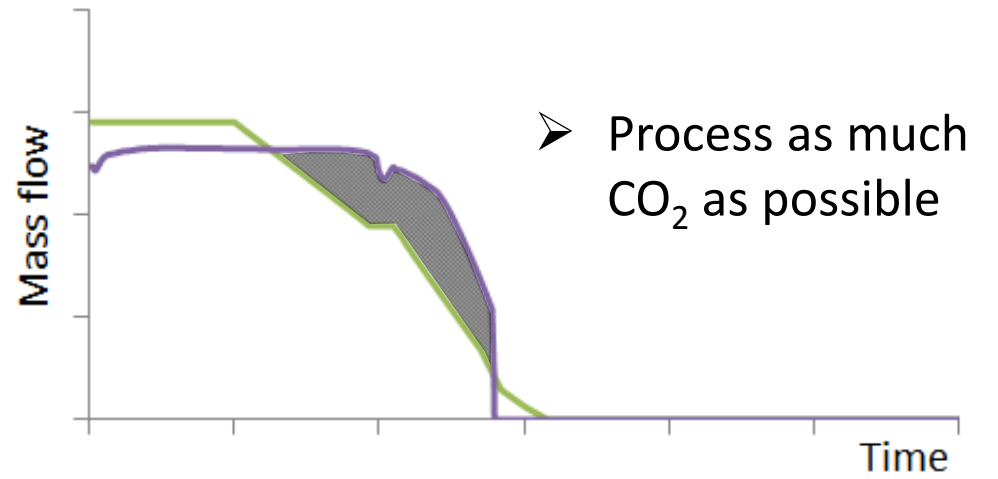
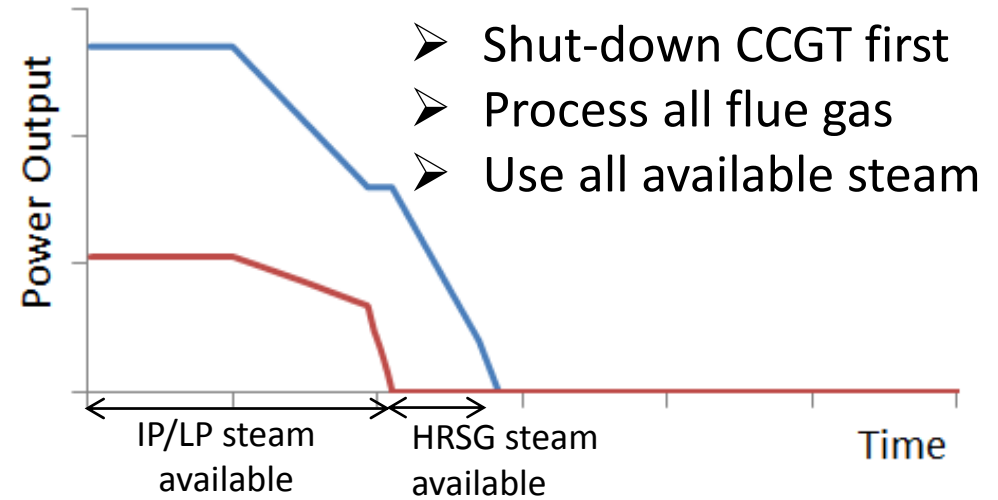
Example: Optimization of shut-down procedure



Normal shut-down



Modified shut-down

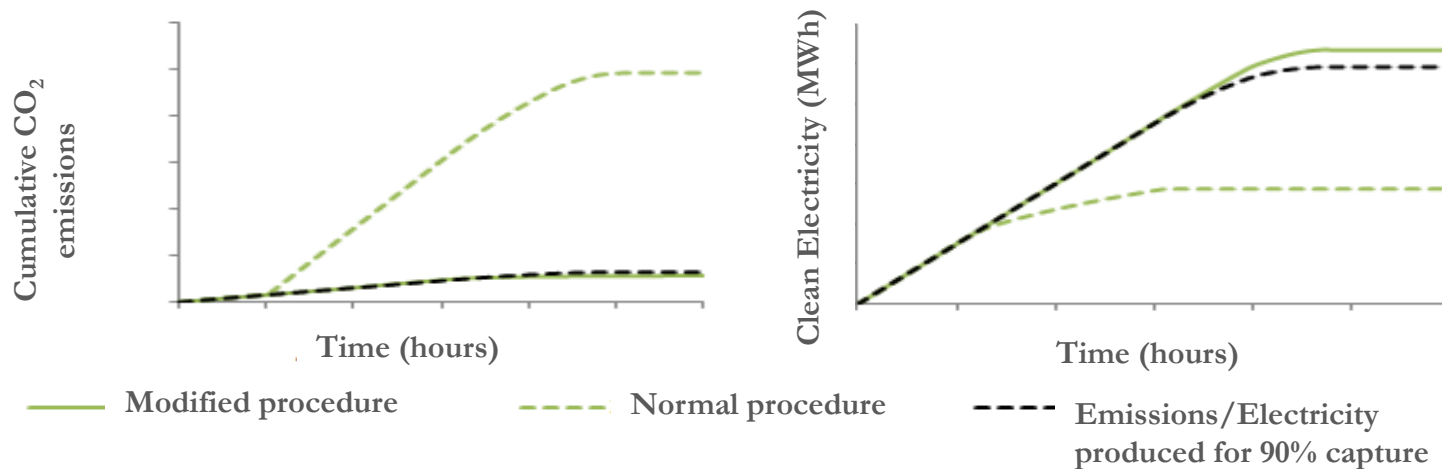


— CO₂ to capture unit — CO₂ to compression unit

Shut-down summary



- It is not necessary to shut down the capture plant before shutting down the power plant
- Modified procedure leads to lower emissions and more clean electricity produced



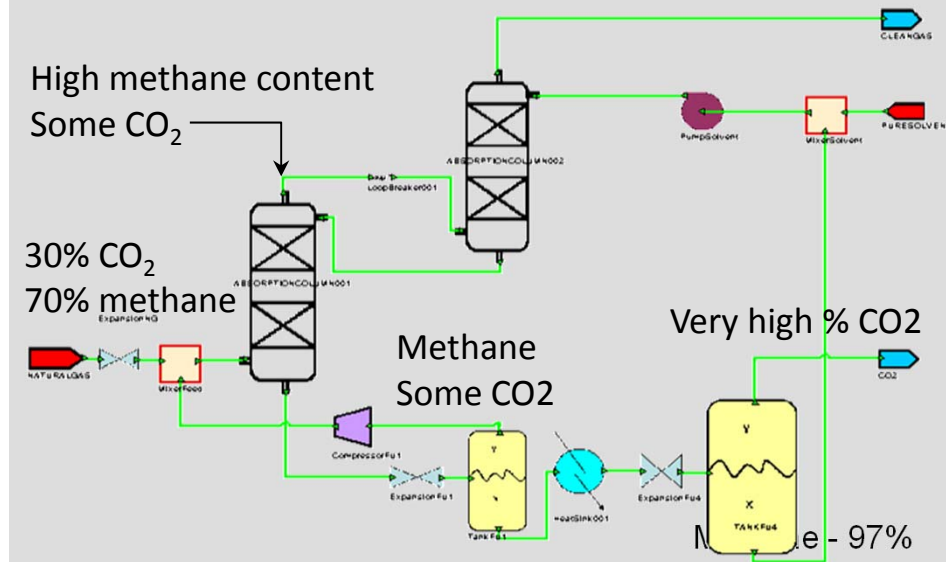
R&D projects



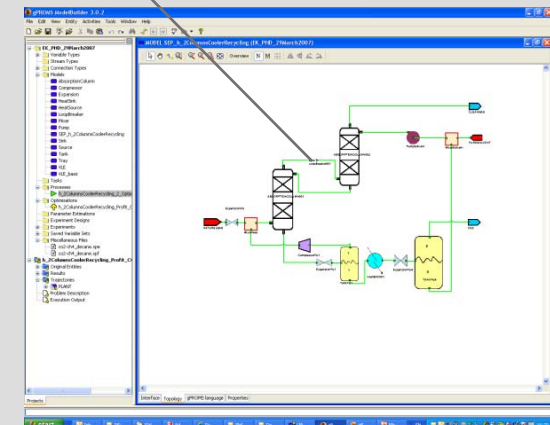
New processes & solvents for carbon capture (Imperial College London, Schlumberger)



- Study:
 - multiple scenarios with various compositions
 - single design that works under all scenarios and conditions
- Simultaneous optimisation of process design and solvent molecular design
- Technologies
 - gPROMS mixed integer optimisation
 - SAFT equation of state



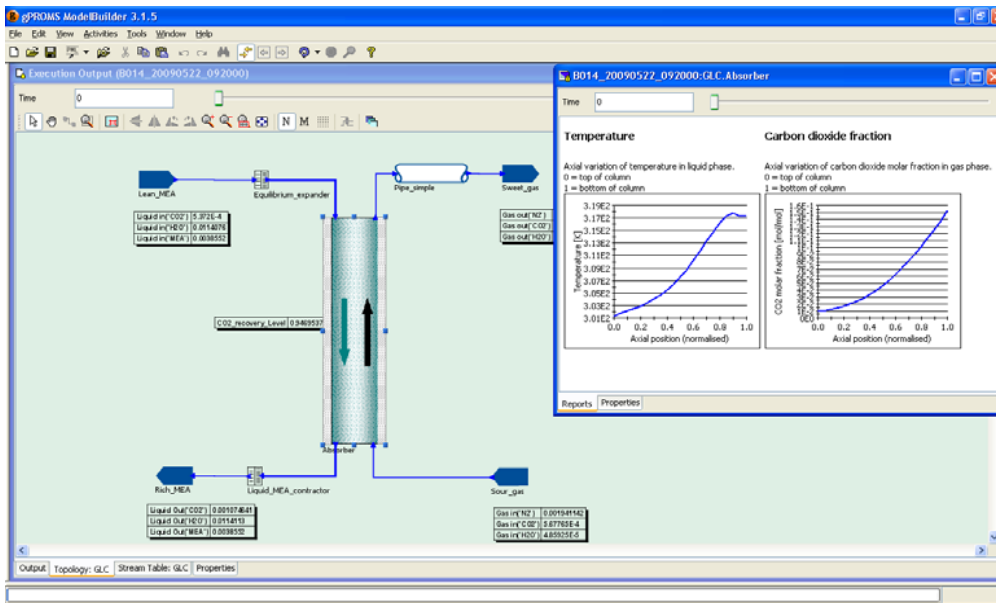
Simultaneous optimisation
of **process design** and
solvent molecular design



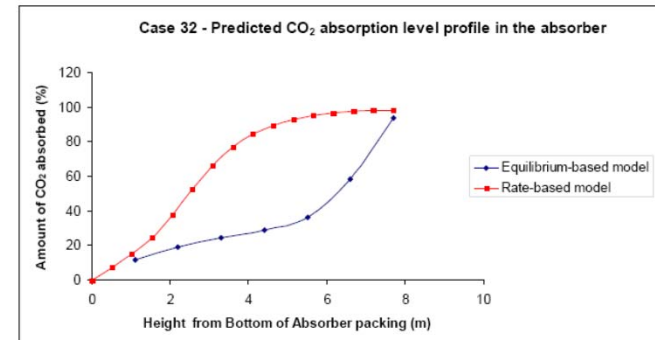
Amine process design (Cranfield, RWE)



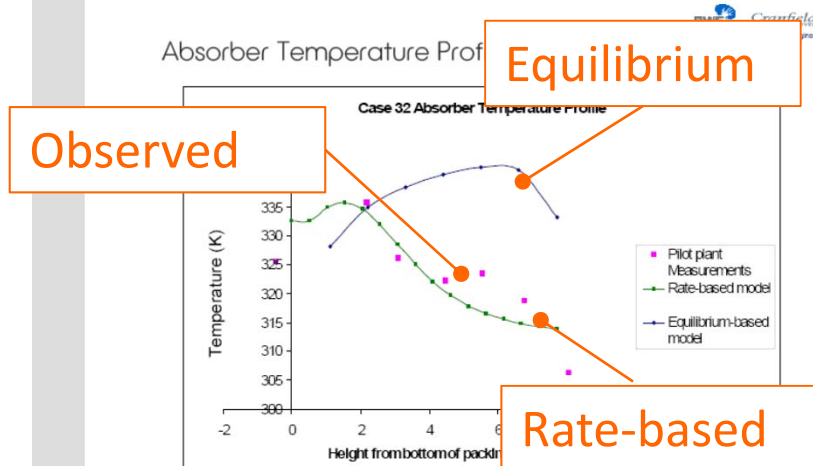
- Importance of **high-fidelity** modelling
 - Rate-based vs. equilibrium methods
 - Completely different results



CO₂ absorption profile predicted by rate- and equilibrium-based models (Case 32)



Absorber Temperature Profile

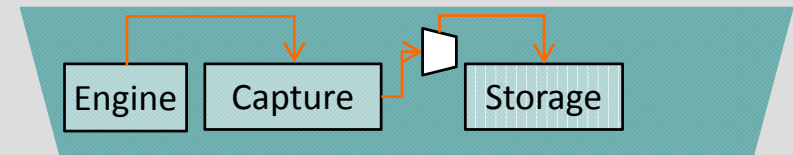


Maritime CCS capture

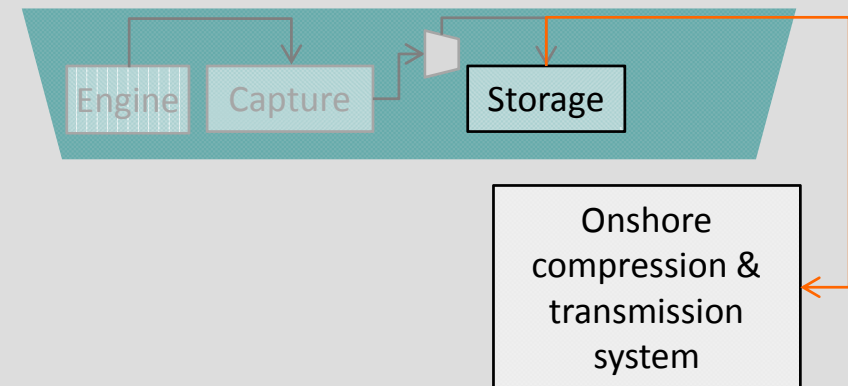


- Significant % of world CO₂ generation is maritime
 - large single-point emissions
- Eurostars project
 - PSE & DNV
 - investigate optimal capture routes
 - process design blueprints
 - safety & operability issues

1. In transit



2. Dock

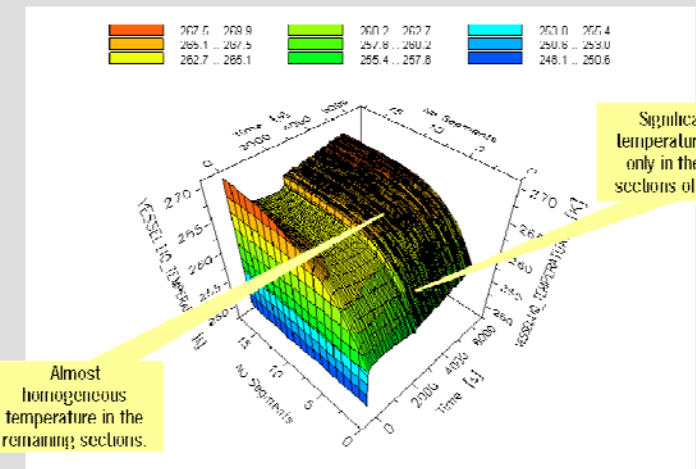
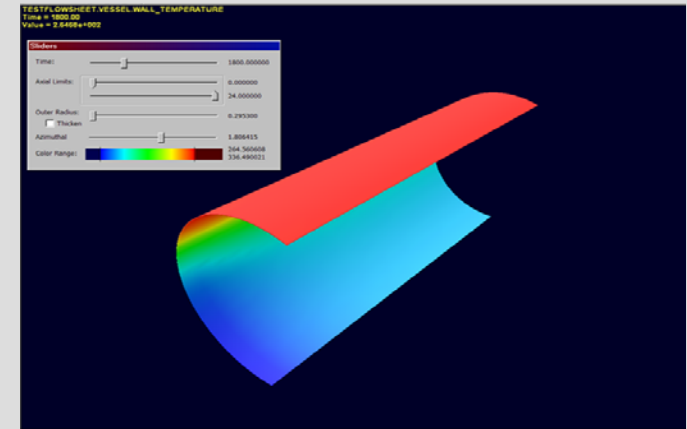
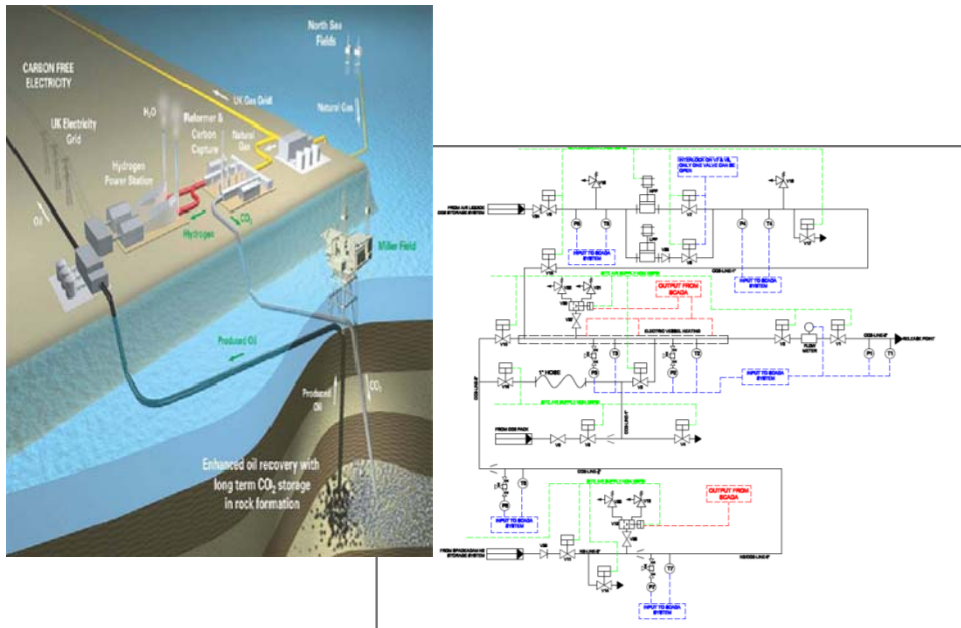


CO₂ compression & transmission (BP, SSE)



BP DF1 project:

- support understanding of different handling scenarios
- example: pipeline temperatures during rapid depressurisation



Applications of gCCS: Case Studies



3. CO₂ Enhanced Oil Recovery Studies (CO₂ EOR)

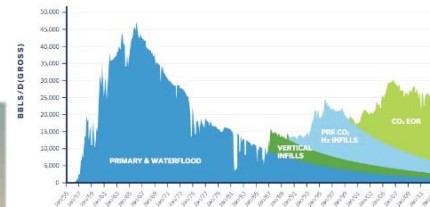
CO₂ Enhanced Oil Recovery: Challenges



Supply vs demand

- Constraints, Costs

Handling of recycled gas before and after breakthrough



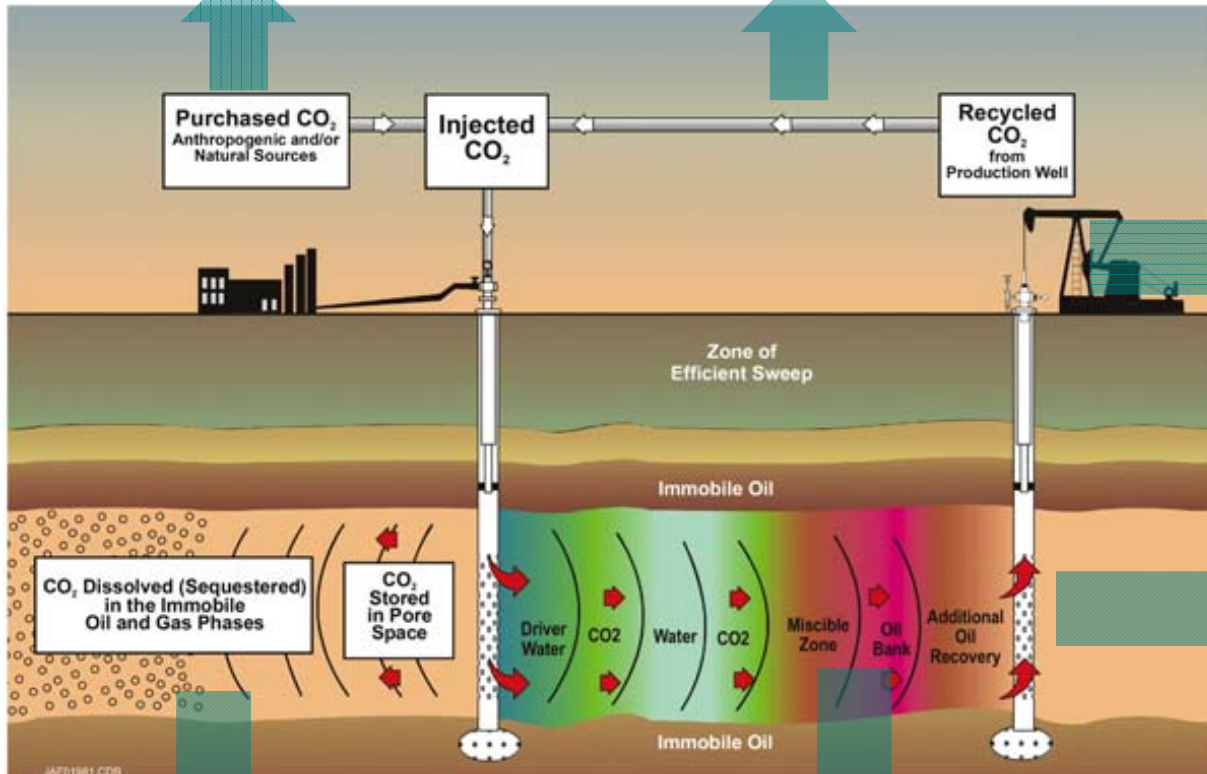
How do I optimize field development schedules?

- Capacity/design/location of facilities?
- Design trade-offs?
- How long can we produce sales gas to spec?

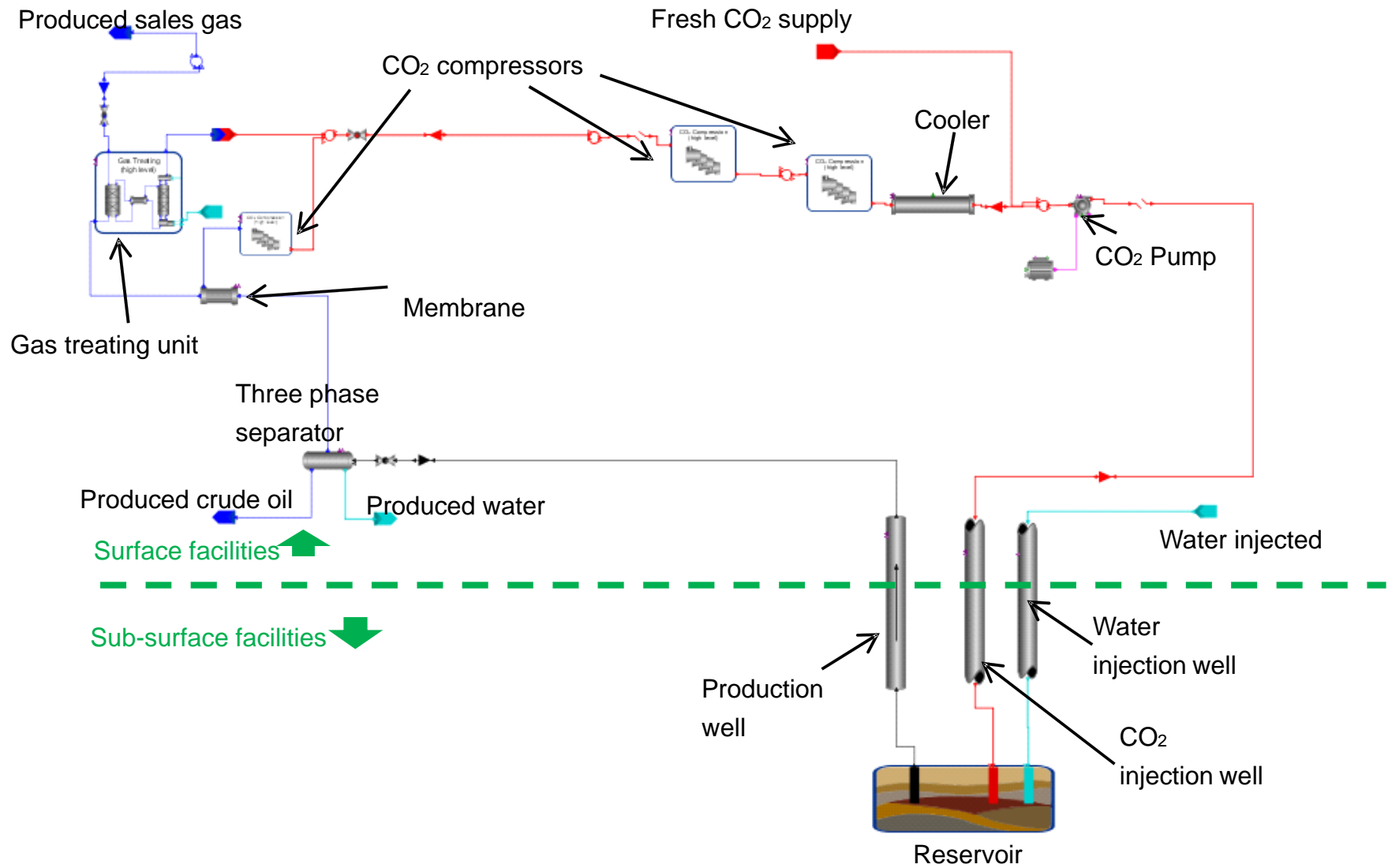
What are the produced fluid composition changes before and after CO₂ breakthrough

- Reservoir dynamic performance?
 - How much oil, water, gas and CO₂ is produced with time?
 - Pressure maintenance requirements?

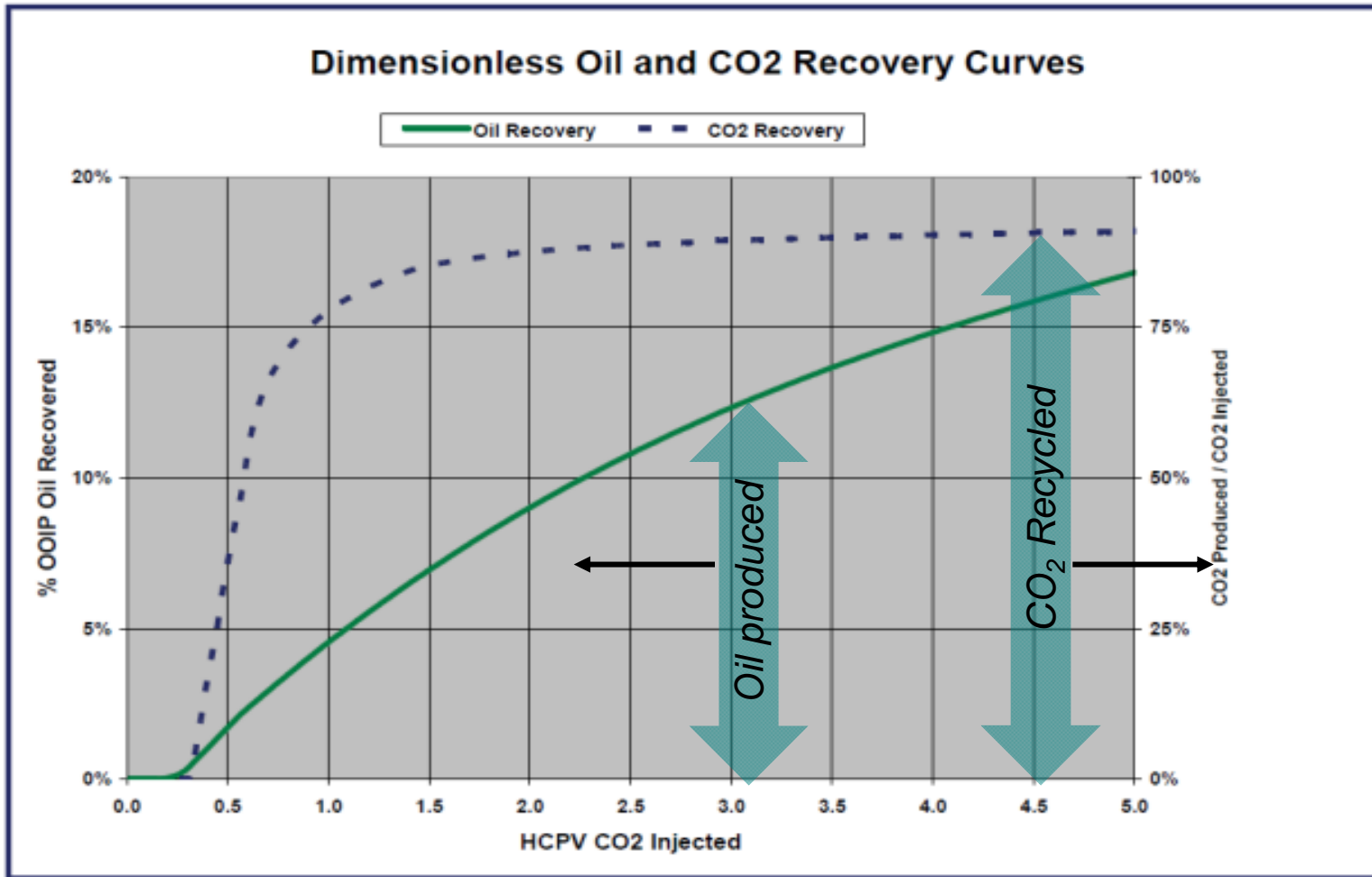
How much CO₂ is stored?



CO₂ EOR Flowsheet in gCCS



Reservoir type curves



Performance predictions from detailed reservoir simulations can be translated to type curves and utilized in gCCS



SPE 144961

Large Scale CO₂ Flood Begins Along Texas Gulf Coast

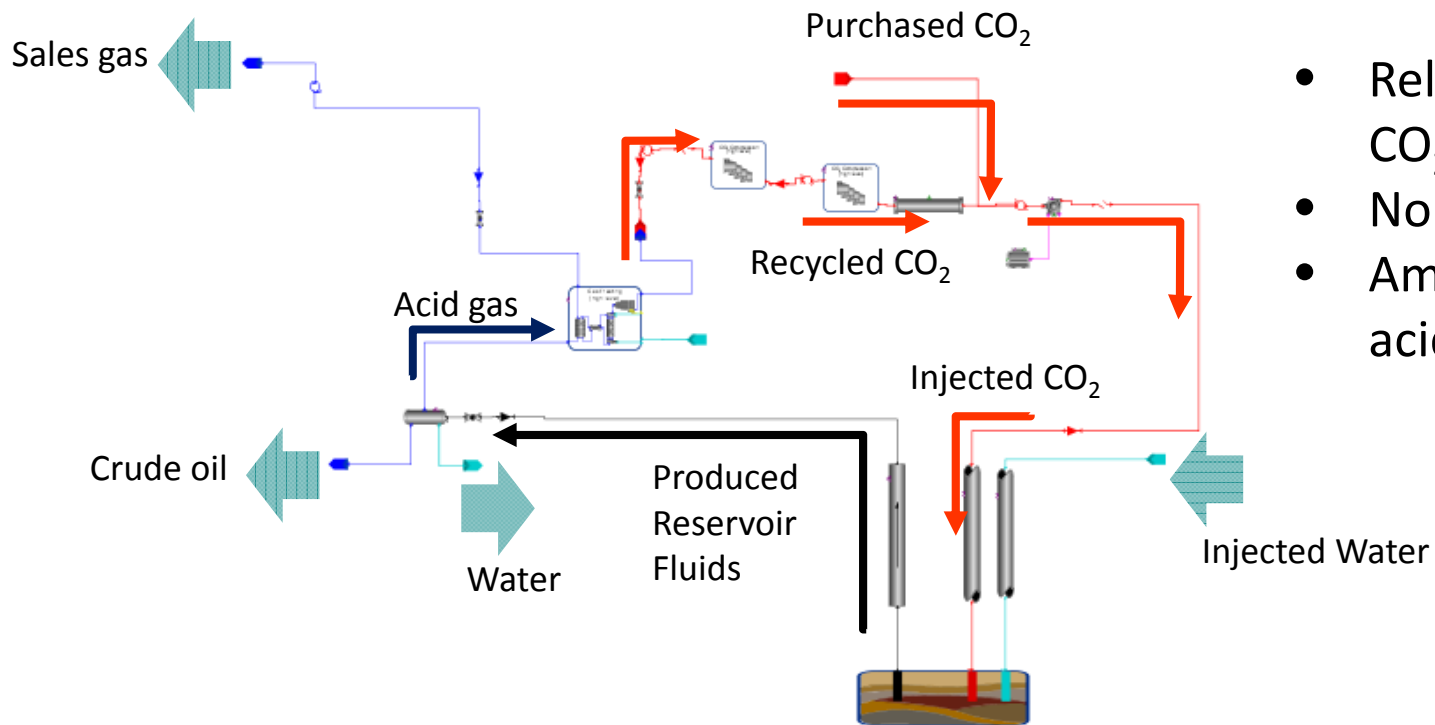
Darrell Davis, SPE, Mark Scott, Kris Roberson and Adam Robinson - Denbury Resources Inc.

Copyright 2011, Society of Petroleum Engineers

This paper was prepared for presentation at the SPE Enhanced Oil Recovery Conference held in Kuala Lumpur, Malaysia, 19–21 July 2011.

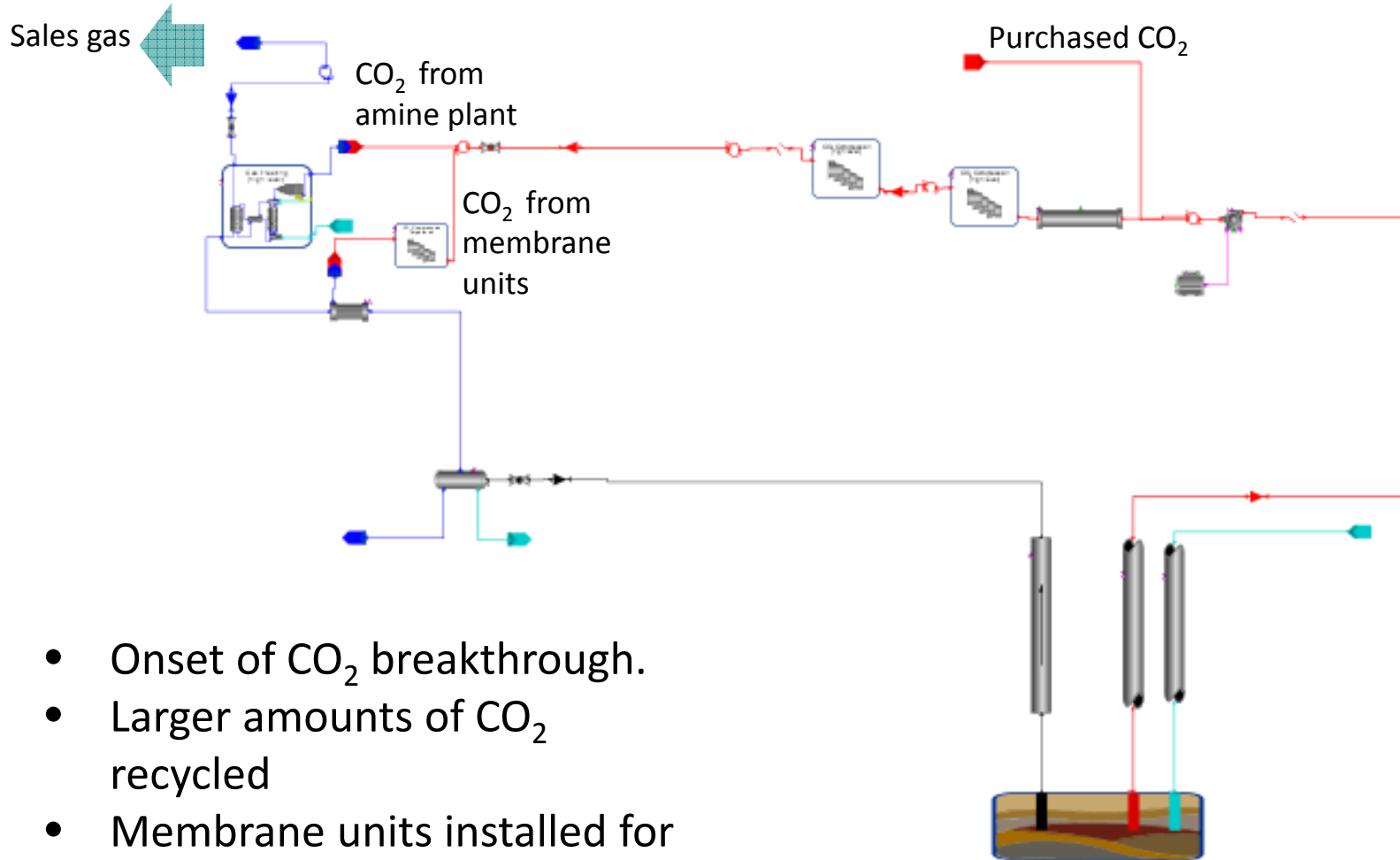
This paper was selected for presentation by an SPE program committee following review of information contained in an abstract submitted by the author(s). Contents of the paper have not been reviewed by the Society of Petroleum Engineers and are subject to correction by the author(s). The material does not necessarily reflect any position of the Society of Petroleum Engineers, its officers, or members. Electronic reproduction, distribution, or storage of any part of this paper without the written consent of the Society of Petroleum Engineers is prohibited. Permission to reproduce in print is restricted to an abstract of not more than 300 words; illustrations may not be copied. The abstract must contain conspicuous acknowledgment of SPE copyright.

Phase 1 operations



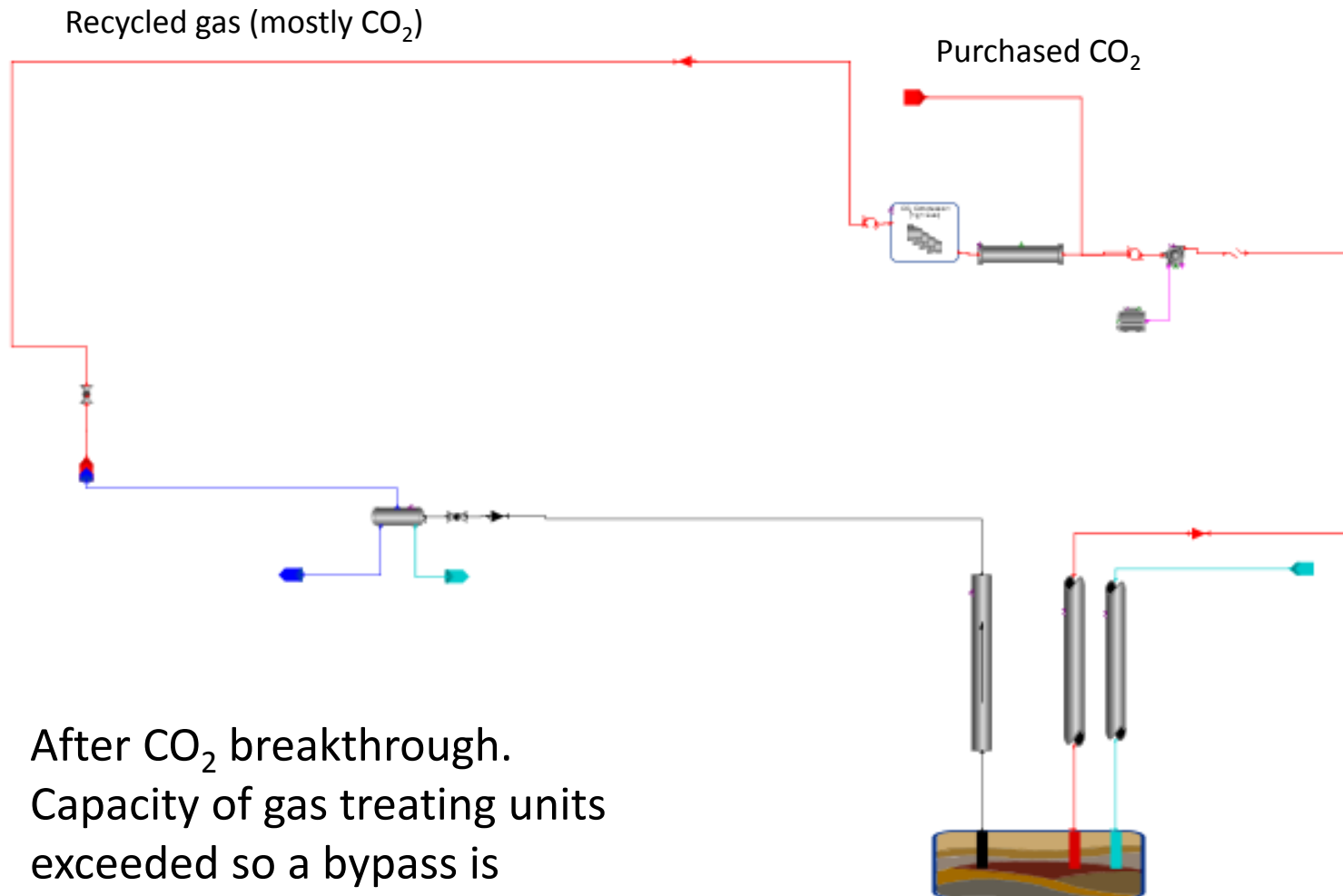
- Before CO₂ breakthrough
- Relatively small amount of CO₂ recycled
- No membrane units
- Amine gas treating removes acid gas to specifications

Phase 2 operations



- Onset of CO₂ breakthrough.
- Larger amounts of CO₂ recycled
- Membrane units installed for additional capacity
- Amine gas treating removes acid gas to specifications

Phase 3 operations

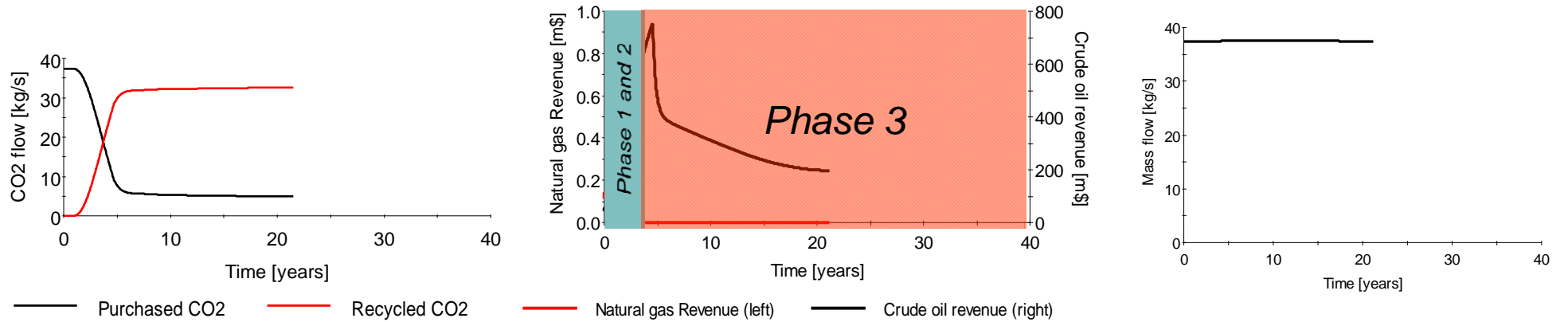


- After CO₂ breakthrough.
- Capacity of gas treating units exceeded so a bypass is established
- CO₂ purity of injected gas drops

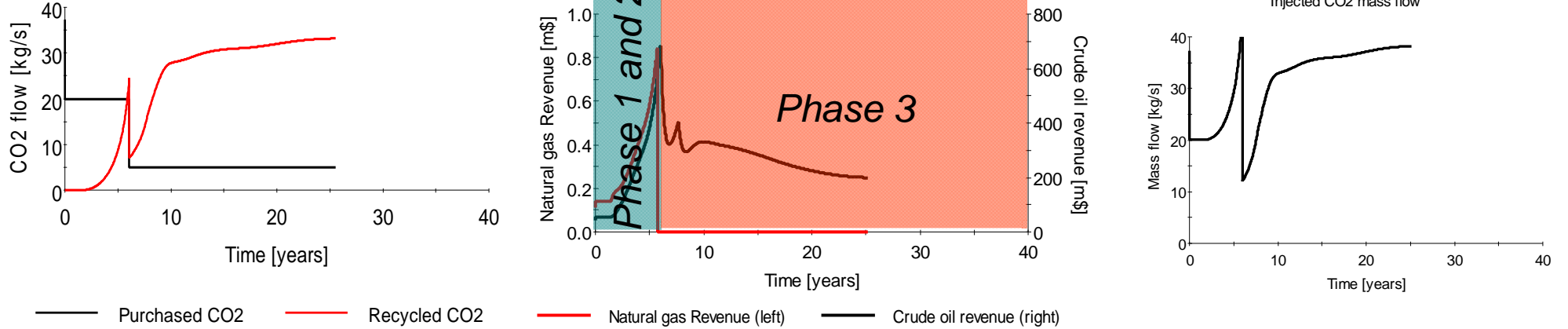
Case Study results – comparing with CO₂ supply constraints



Unconstrained supply

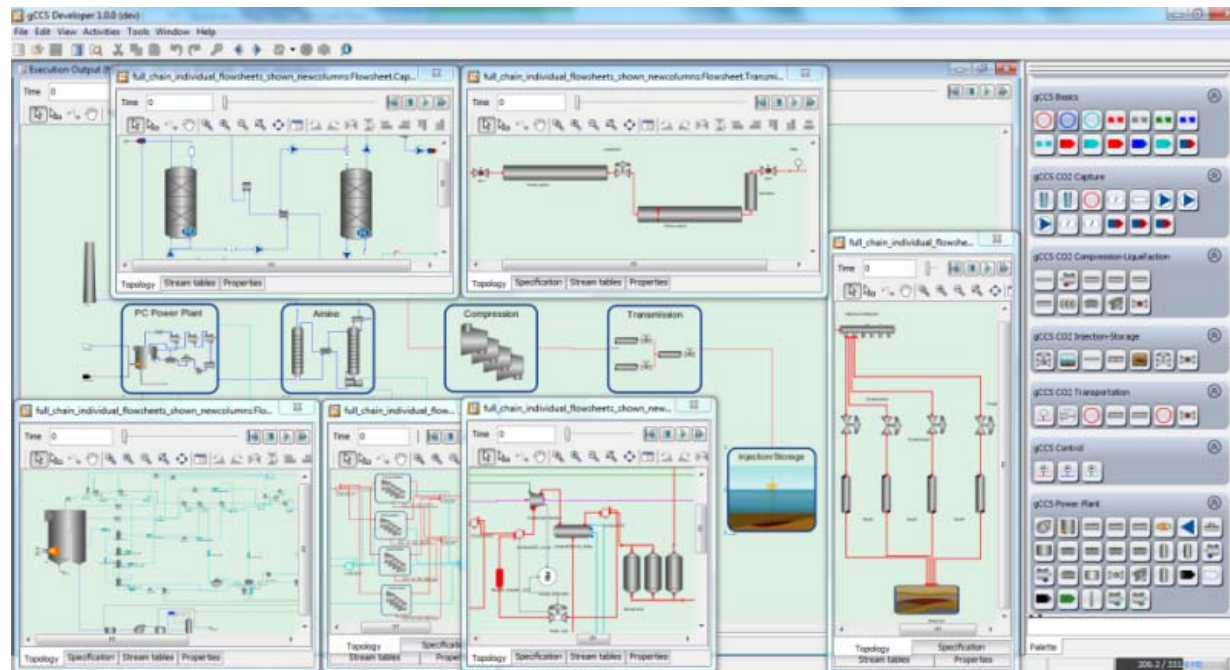


Constrained supply



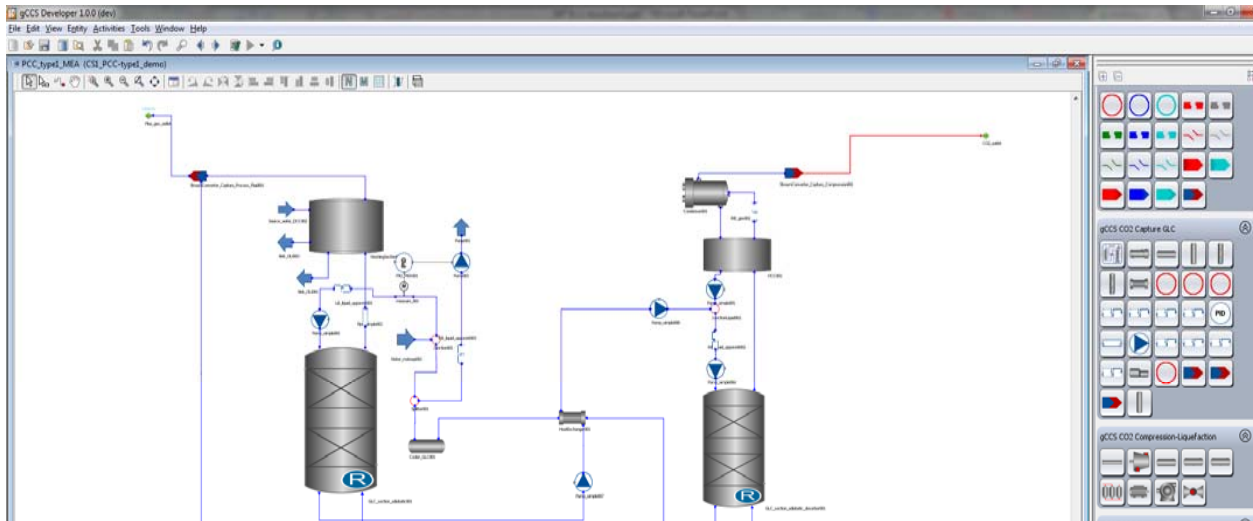
■ System integration is crucial

- Assess heat integration options to reduce parasitic load
- Identify opportunities to reduce cost of capture, e.g. use of let-down steam in post-combustion capture
- Test alternative capture technologies and assess their suitability for retrofitting existing plants



Improving commercial viability

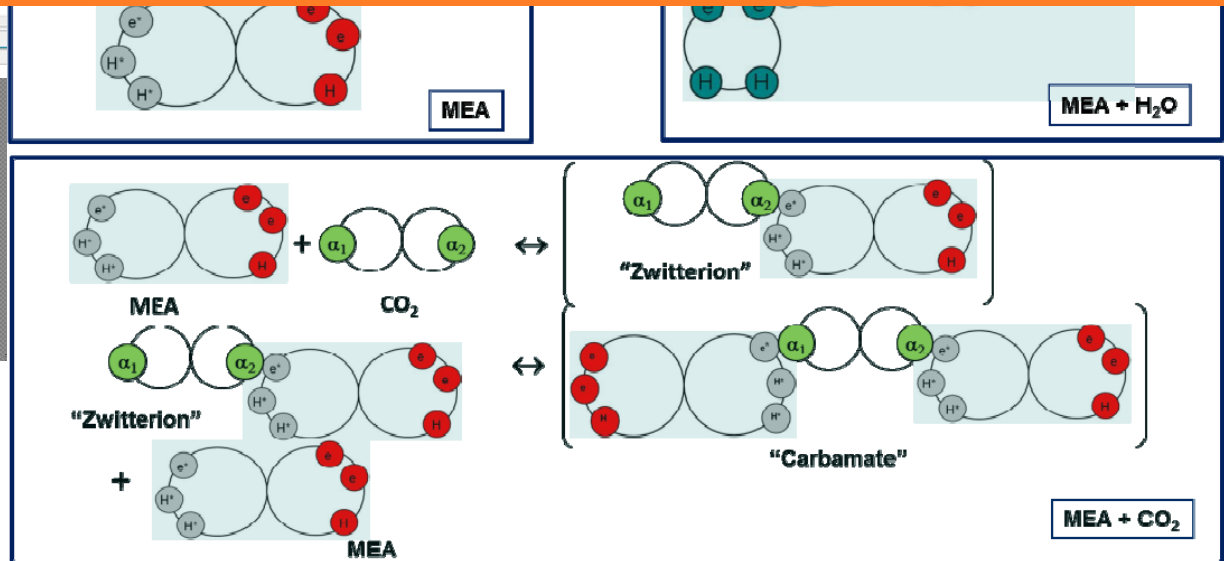
Cost reductions



Process design
 Configuration
 Equipment size
 Heat integration
 ...
 Process operation
 Solvent loading
 Flowrates
 Pressures, temperatures
 ...

APM enables the simultaneous optimisation of all these aspects achieving more economical solutions

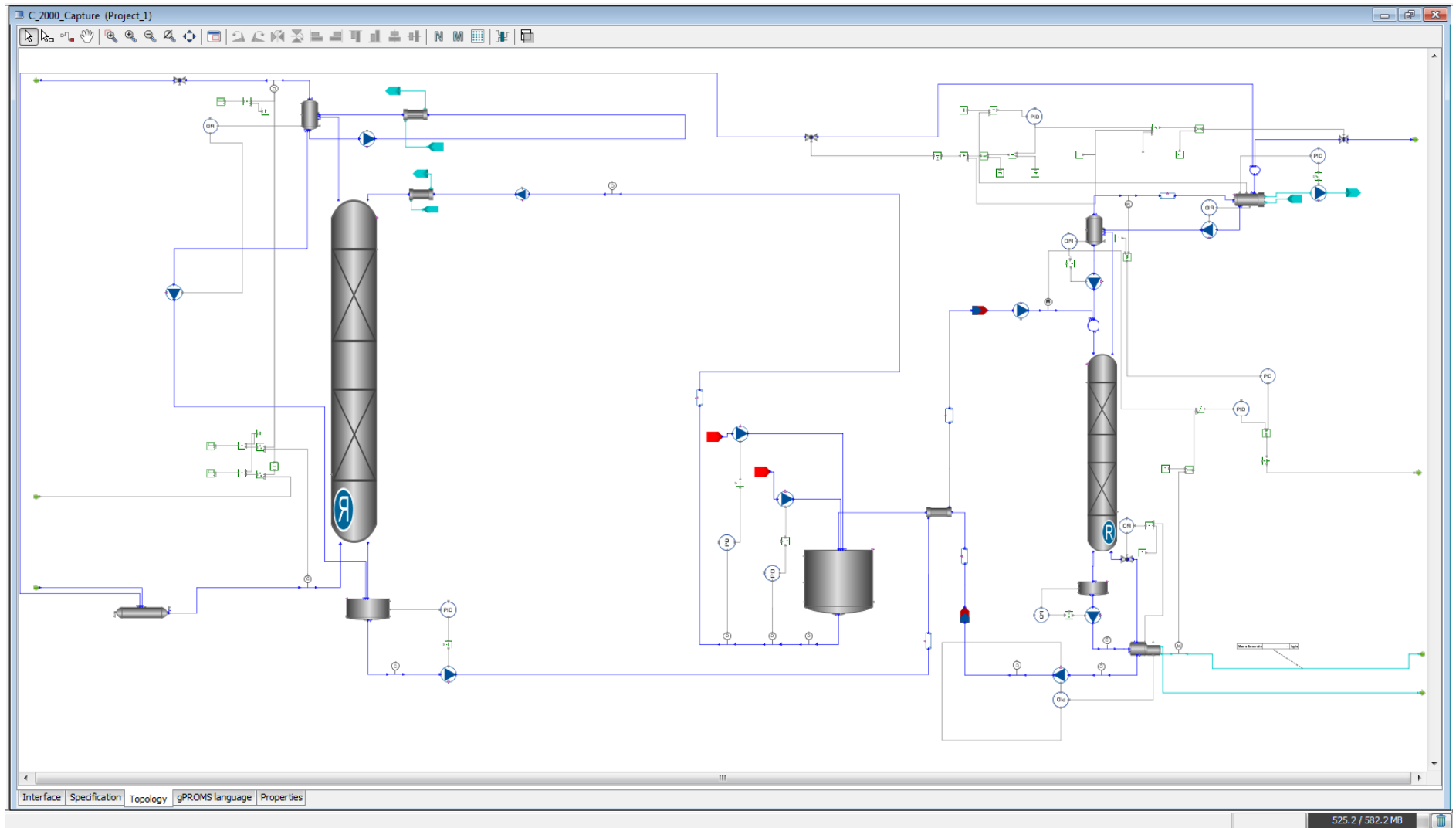
Solvent design/development
 Screening of candidates
 New molecules (group contribution method)
 New mixtures



Improving commercial viability Cost reductions



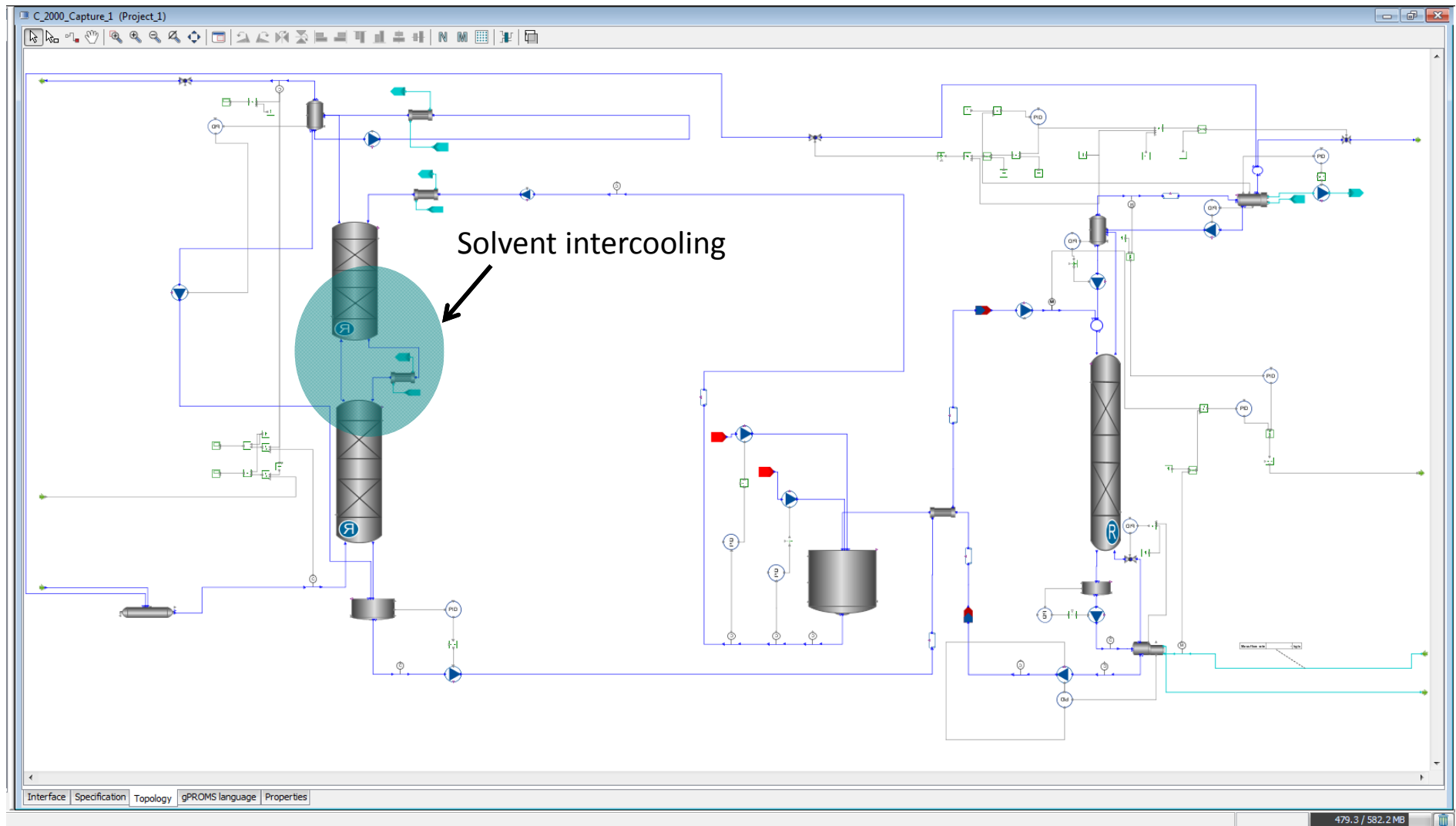
■ Process design – alternative solvent-based PCC configurations



Improving commercial viability Cost reductions



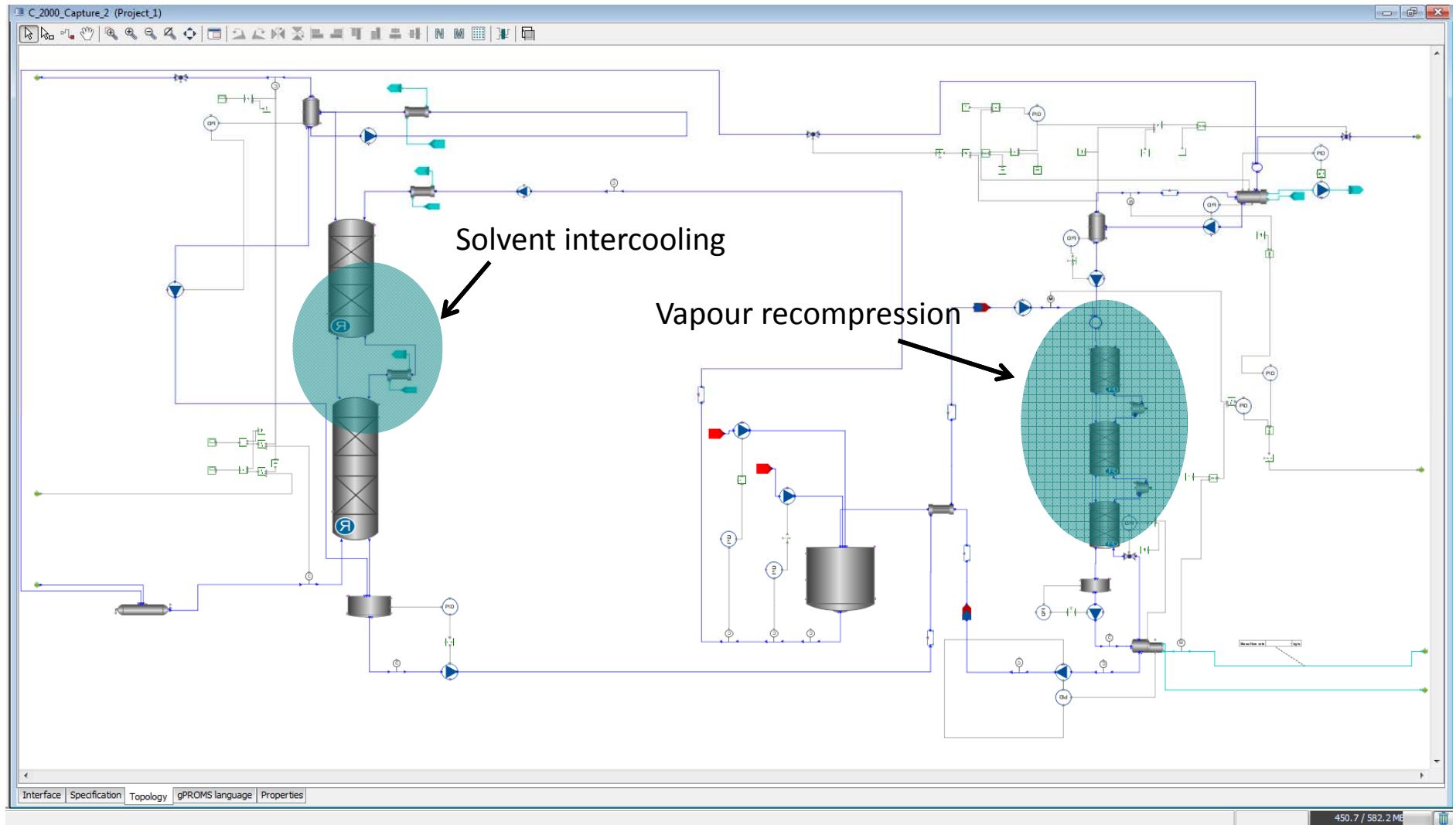
■ Process design – alternative solvent-based PCC configurations



Improving commercial viability Cost reductions



■ Process design – alternative solvent-based PCC configurations



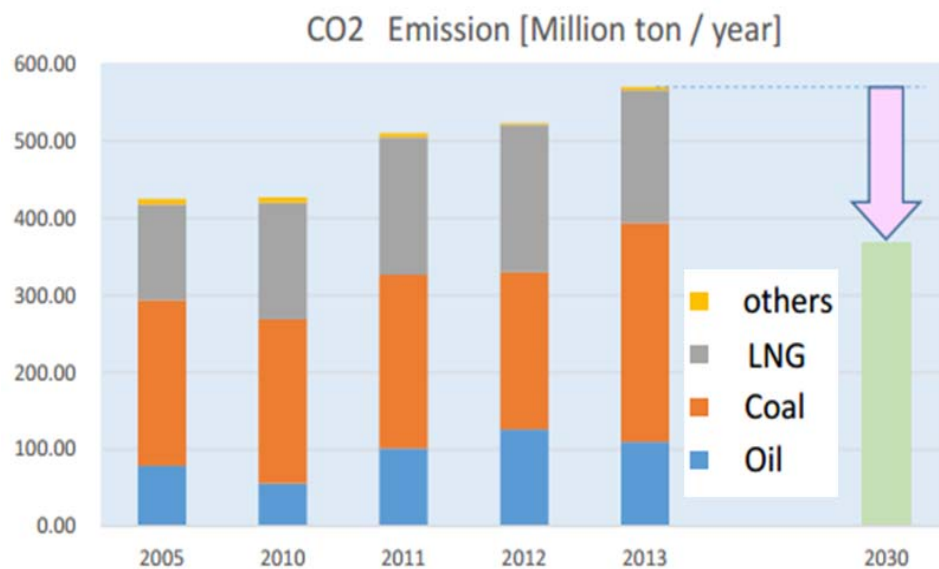
CCS in Japan



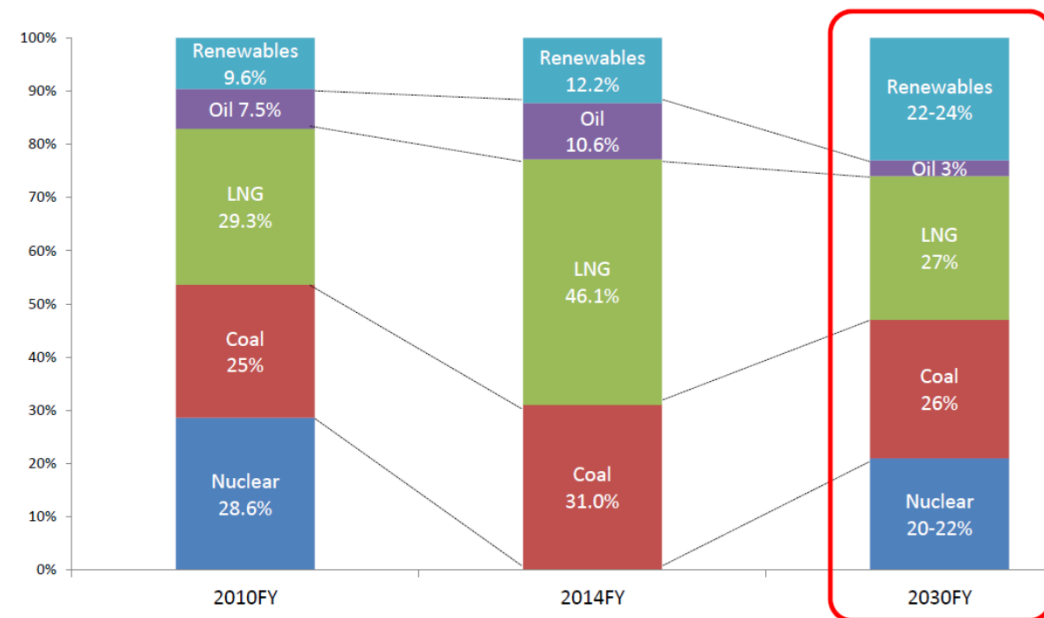
Plan for emissions reduction in Japan (I)



- 26% Total Emission Reduction from 2013 level
- Translates for the Power Generation sector to a reduction of 35% from 2013 level
- Reductions achieved primarily by switching from LNG/Oil/Coal plants to Nuclear & Renewables generation



quoted from materials of the Federation of Electric Power Companies of Japan, issued in July 2015

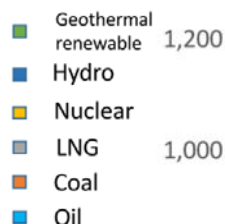


Source: Yamazaki, T., Director for Electricity Market Reform, Ministry of Economy, Trade and Industry, July 2015

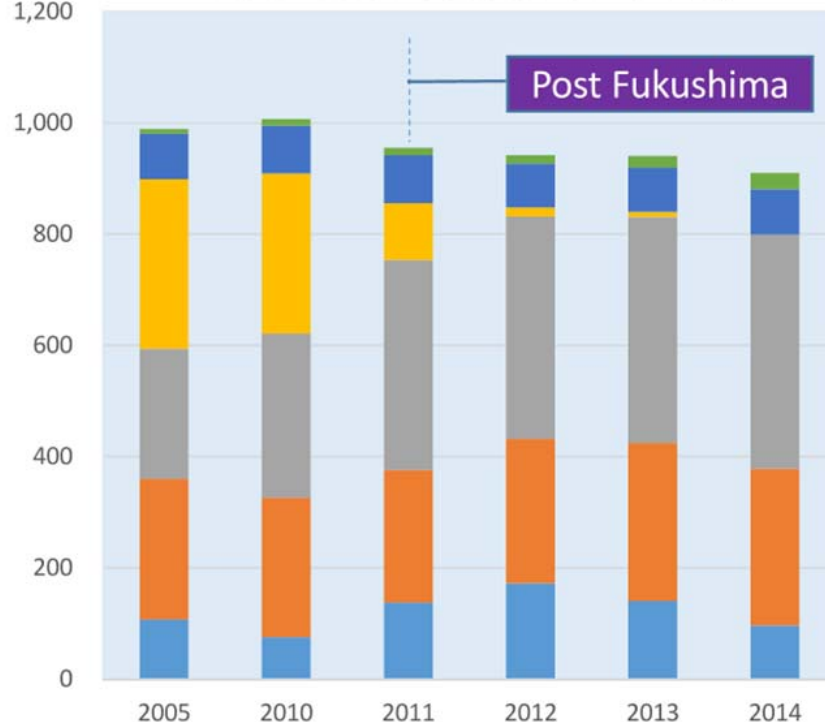
Uncertainty affecting the targeted reductions



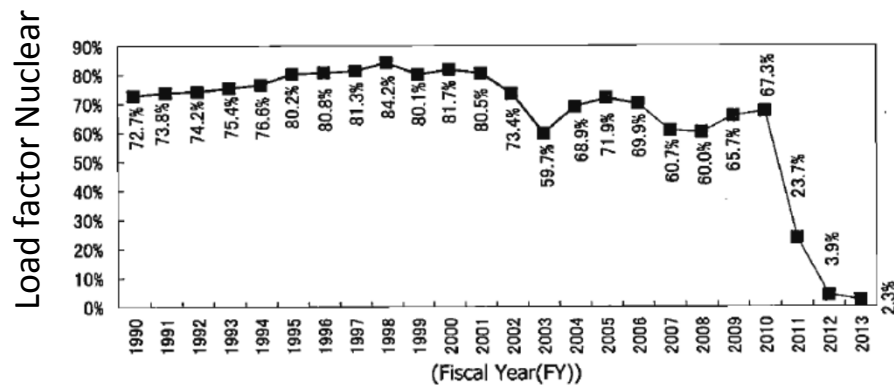
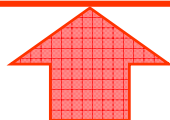
- Public acceptance of nuclear power post-Fukushima
 - One nuclear power unit out of 44 restarted in Aug 2015
 - 8.75GW of coal-fired power plants planned



Total Power Generation [TWh]



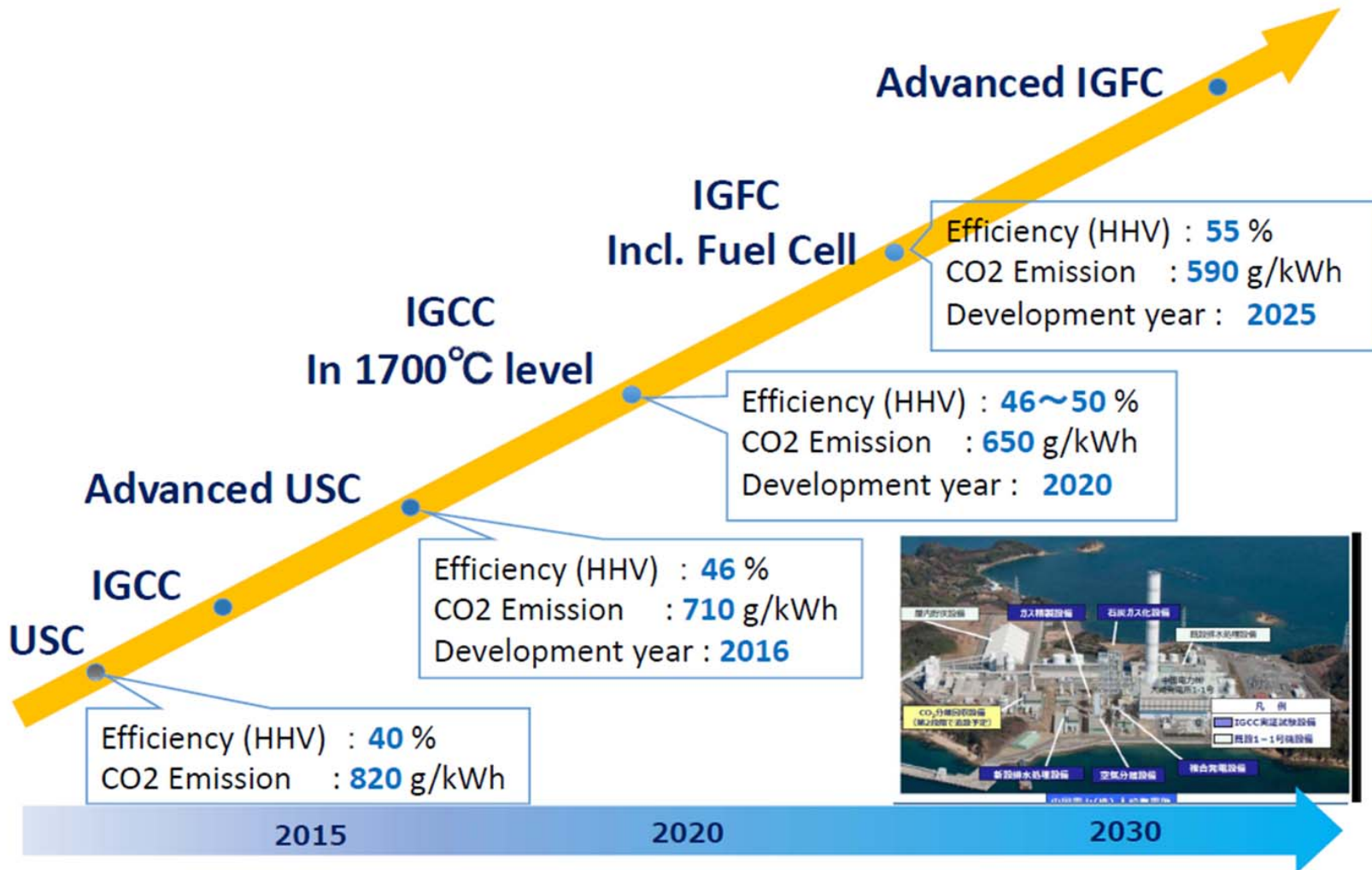
- Development of low-carbon fossil generation technologies
 - Efficiency increases in fossil fuel generation
 - Carbon Capture & Storage



(Source) The Federation of Electric Power Companies of Japan

Plan for emissions reduction in Japan (II)

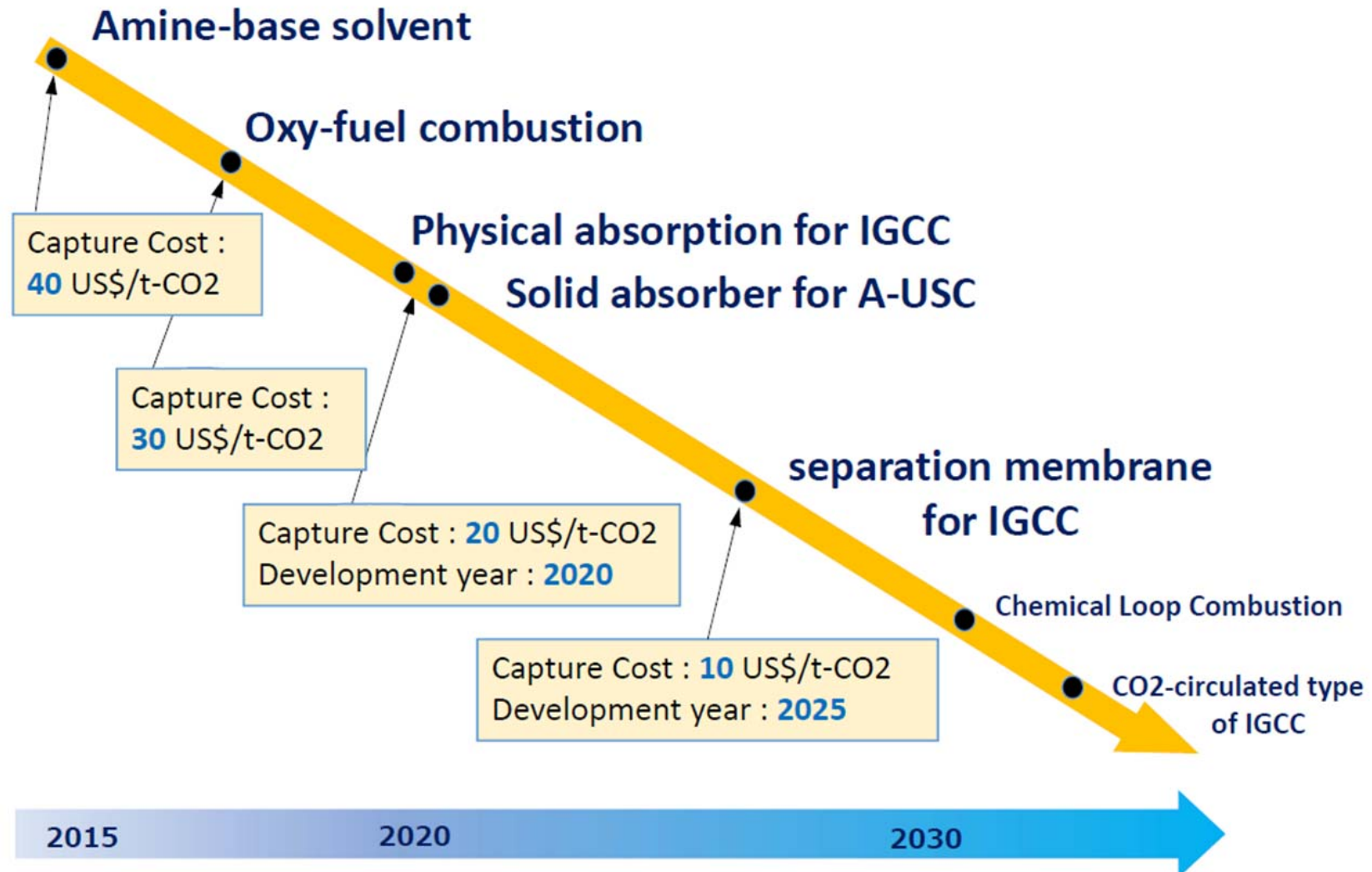
- Drive for higher efficiency in coal-fired power generation



Plan for emissions reduction in Japan (IV)



■ Roadmap for CCS in Japan



Plan for emissions reduction in Japan (VI)

Challenges for CCS: Cost



- Outlook 2030 – there is hope!
 - Figures from Ministry of the Environment in Japan are equally optimistic

Type	Generating Capacity [MW]	Transport Distance [km]	CCS Cost [US\$/t-CO ₂]	Electricity Cost [US\$/kWh]		
				Generation	CCS	Total
Super Critical Pressure Coal-Fired (SC)	750	185	90	0.085	0.086	0.172
		600	97		0.093	0.179
		970	103		0.099	0.185
Ultra Super Critical Pressure Coal-Fired (USC)	750	185	91	0.079	0.075	0.154
		600	99		0.080	0.160
		970	105		0.086	0.165
Integrated Gasification Combined Cycle (IGCC)	750	185	78	0.099	0.073	0.172
		600	85		0.079	0.179
		970	91		0.085	0.184
Natural Gas Combined Cycle (NGCC)	750	185	124	0.092	0.045	0.138
		600	131		0.047	0.140
		970	137		0.050	0.142

Source: Sekiya, T., Director Low-Carbon Society Promotion Office, Ministry of the Environment (MOE), Jan 2016

* Exchange rate: USD/JPY = 100

- How to achieve those cost reductions...
 - with only limited experience of large-scale integrated projects?
(so far only SaskPower's Boundary Dam)

 - while making the most efficient use of technology development funds?
(e.g. by supporting most promising technologies)

System- and process **modelling is** one of the
key ingredients for success