APM 2013

The Advanced Process Modelling Forum

17-18 April 2013, London

PSE

Whole-chain system modelling for CCS

Accelerating deployment and managing risk

Alfredo Ramos – Head of CCS & Power Business

Introduction to systems modelling - overview

- Objectives of this presentation
- CCS System Modelling Tool-kit project
- gCCS overview & demonstration
  - Model libraries
  - Physical properties
  - Interfaces

Objectives

- Provide an introduction to the ETI's CCS System Modelling Tool-kit (SMTK) project
  - Context:
    - Key role played by model-based approaches in reducing technological and financial risk
    - Why is it necessary to adopt a system-wide approach covering the whole CCS chain?
  - Requirements & timelines
- Demonstrate gCCS's capabilities
  - Tool-kit's approach to whole- and partial chain modelling
  - Current functionality (available models, interfaces, etc.)
  - Examples for pulverised-coal power plants, compression, transmission & injection

…and whole chain simulation!

CCS system modelling tool-kit project

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Energy Technologies Institute (ETI)

- Public-private partnership between global industries and the UK Government set up with the objectives of
  - ensuring clean, secure and affordable energy supplies are available to power everyday living and business
  - reducing greenhouse gas emissions to tackle the effects of climate change
- ETI members

corporate

public institutions

- The ETI is not a grant-giving body, but makes targeted investments in key technologies that will help the UK meet its’ legally binding 2050 targets

The CCS landscape – stakeholders

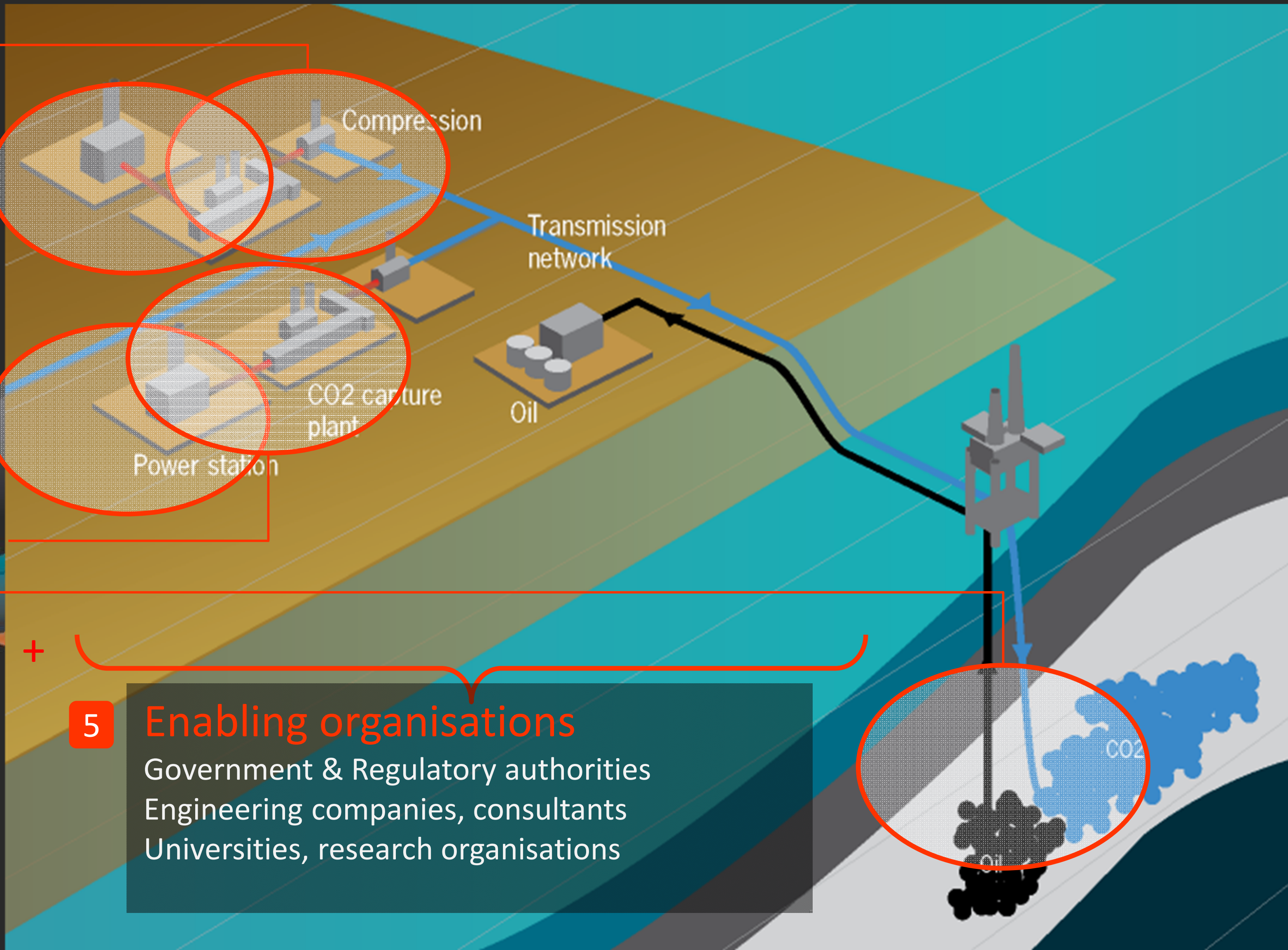
Compression & transmission 3

Industrial gas companies 2

Power generators 1

Process providers 2

Storage providers 4



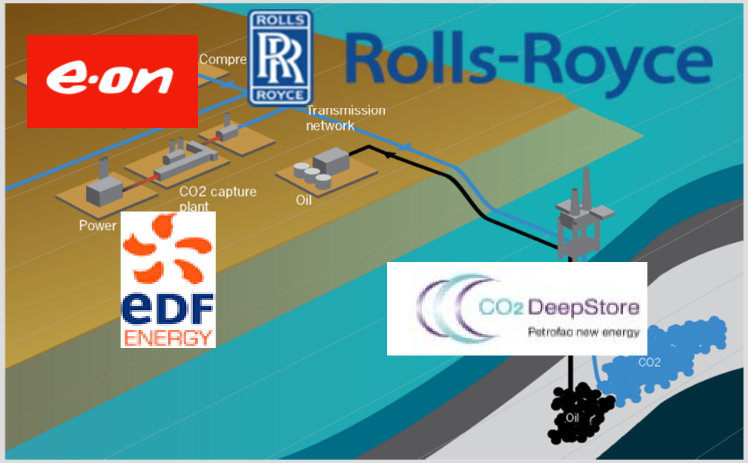
System-wide modelling key enabling technology for CCS: benefits

- 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 **interaction** 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

→ **Manage complexity and risk at a multi-scale, network-wide level**

System-wide modelling: Key enabling technology for CCS

- **CCS System Modelling Tool-kit Project**
  - Energy Technologies Institute (ETI) £3m project
  - E.ON, EDF, Rolls-Royce, Petrofac/CO2DeepStore, PSE, E4tech



gPROMS modelling platform technology & expertise

Management

→ Create a commercially available product
- built on PSE's gPROMS platform
- High-fidelity system-wide CCS modelling
- Toolbox and ecosystem

Goal

- A tool that **goes a long way towards** addressing the challenges in the commercialisation of CCS
- High-quality, validated **first-principles models**
  - common model basis – consistency and quality
  - steady state and dynamics within same framework
  - consistent, accurate **physical properties** for near-pure CO_2 mixtures and amine-based solvents
- A 'common language' for **industry and academic** stakeholders
  - reduces duplication in modelling work (both industry & academia)
  - provides a custom modelling language for additional components
  - incorporate **3rd-party models**

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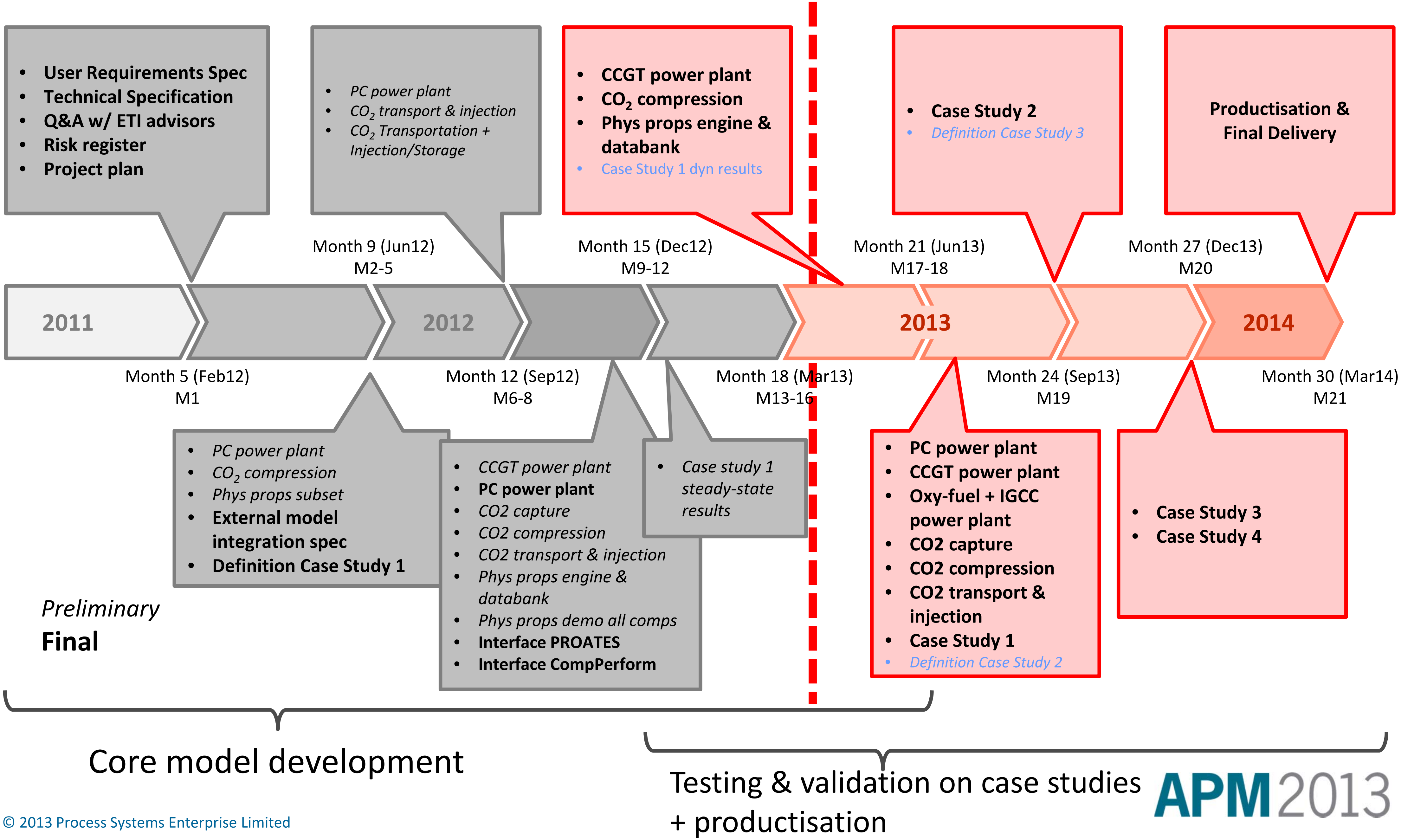
Tool-kit components

Model libraries

- Model libraries
  - Power generation
  - Solvent-based CO_2 capture
  - Compression & Liquefaction
  - Transportation
  - Injection in sub-sea storage
- Physical properties
  - Tailored to each sub-system in the CCS chain
- Interfaces to 3rd party modelling packages
- Detailed documentation of all tool-kit components

Timelines



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Tool-kit components / functionality

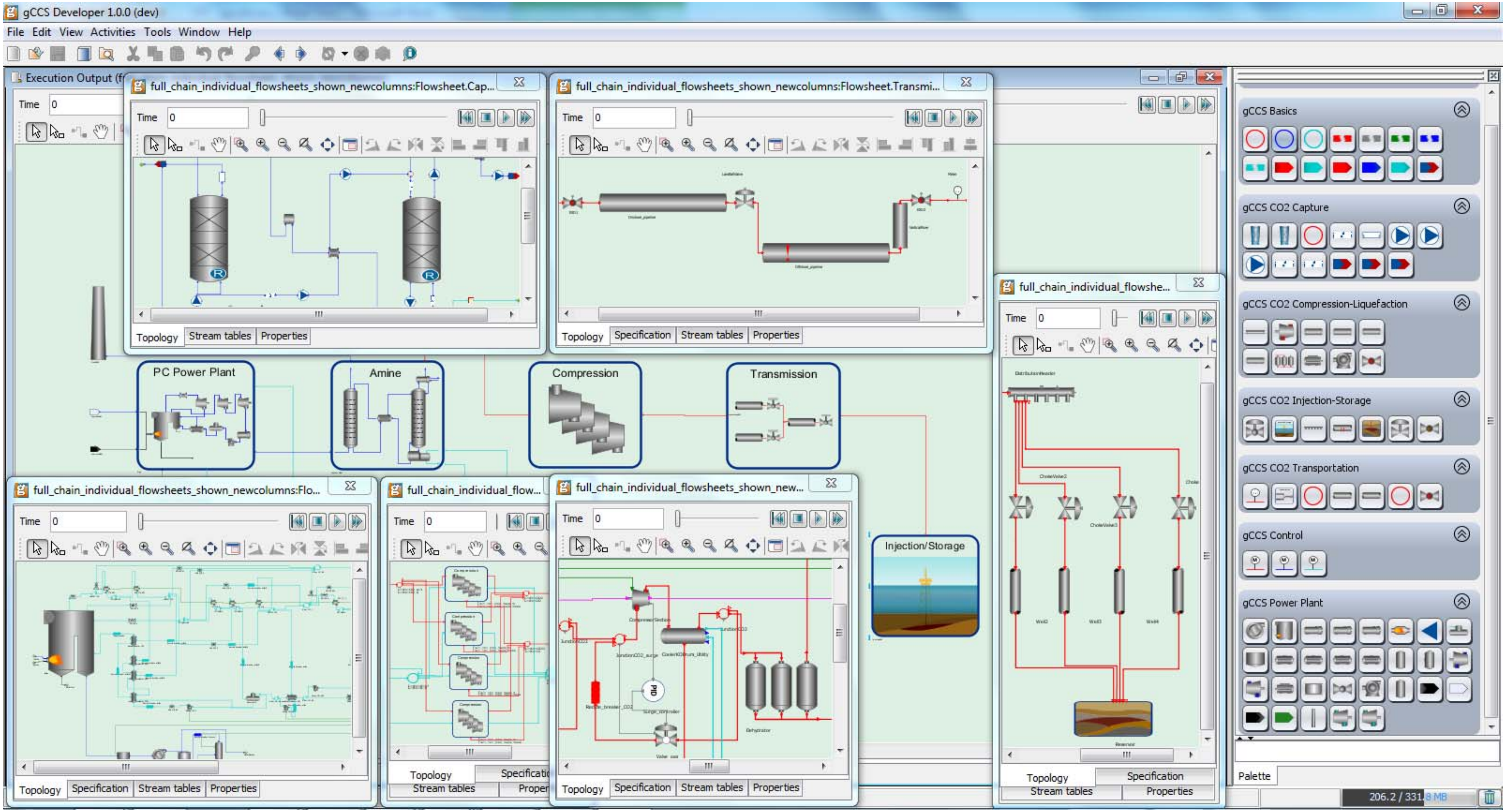
Model libraries

Physical properties

Interfaces

Tool-kit components

Model libraries – Overview



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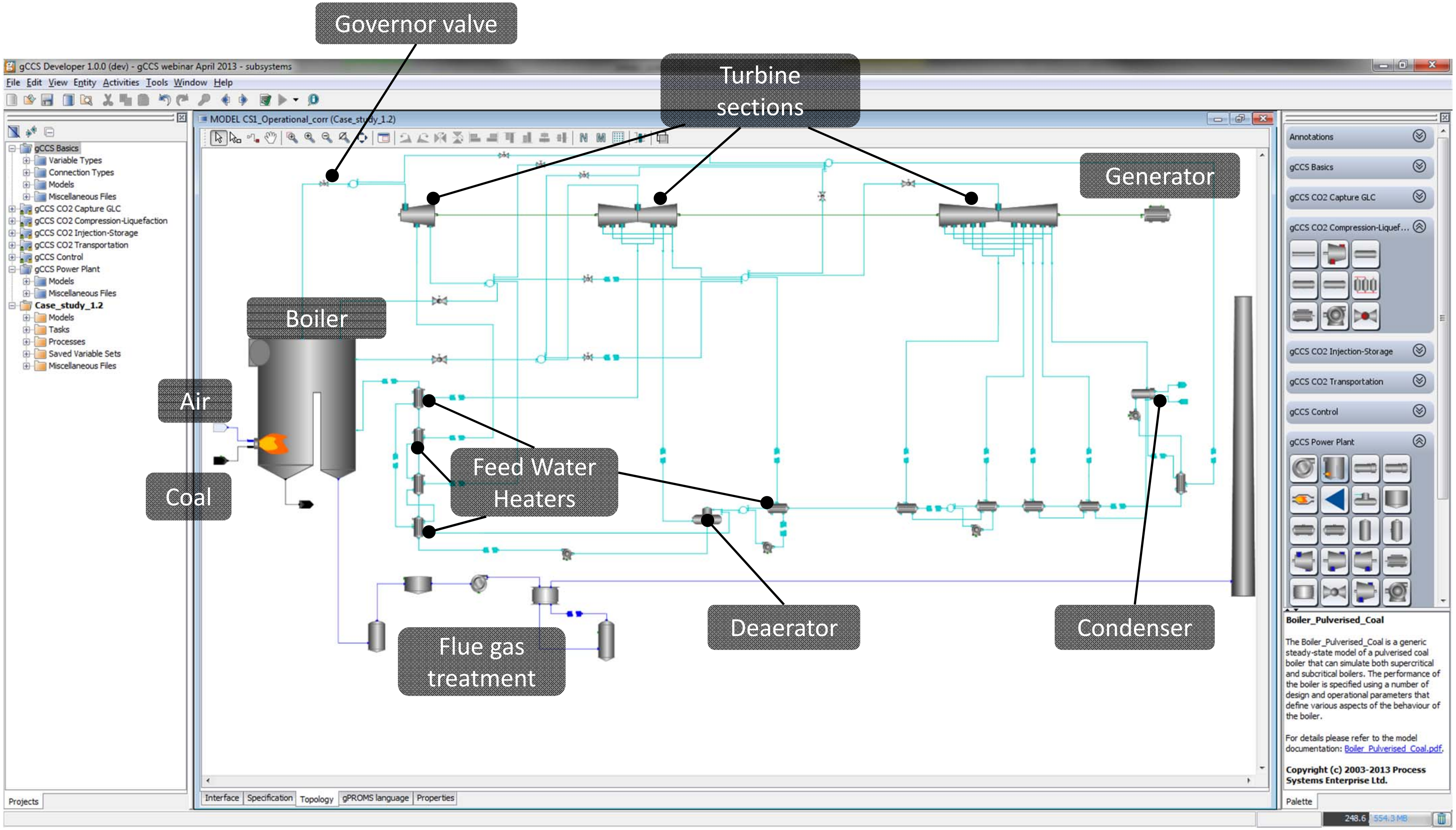
Tool-kit components

Model libraries – Overview

- Power generation
  - Conventional (coal-fired, CCGT) and non-conventional (oxy-fuel, IGCC)
- Solvent-based CO_2 capture
  - both chemical and physical processes
- Compression & Liquefaction
  - multi-stage, multi-section compressors, surge control valves, drives, etc.
- Transportation
  - on- and off-shore pipelines
- Injection in sub-sea storage
  - distribution headers, well connections, reservoir, etc.

Tool-kit components

Model libraries – Power plant



Complex flowsheet with > 10 recycles & a closed loop:

→ Component-specific initialisation procedures ensure convergence **without SVS**

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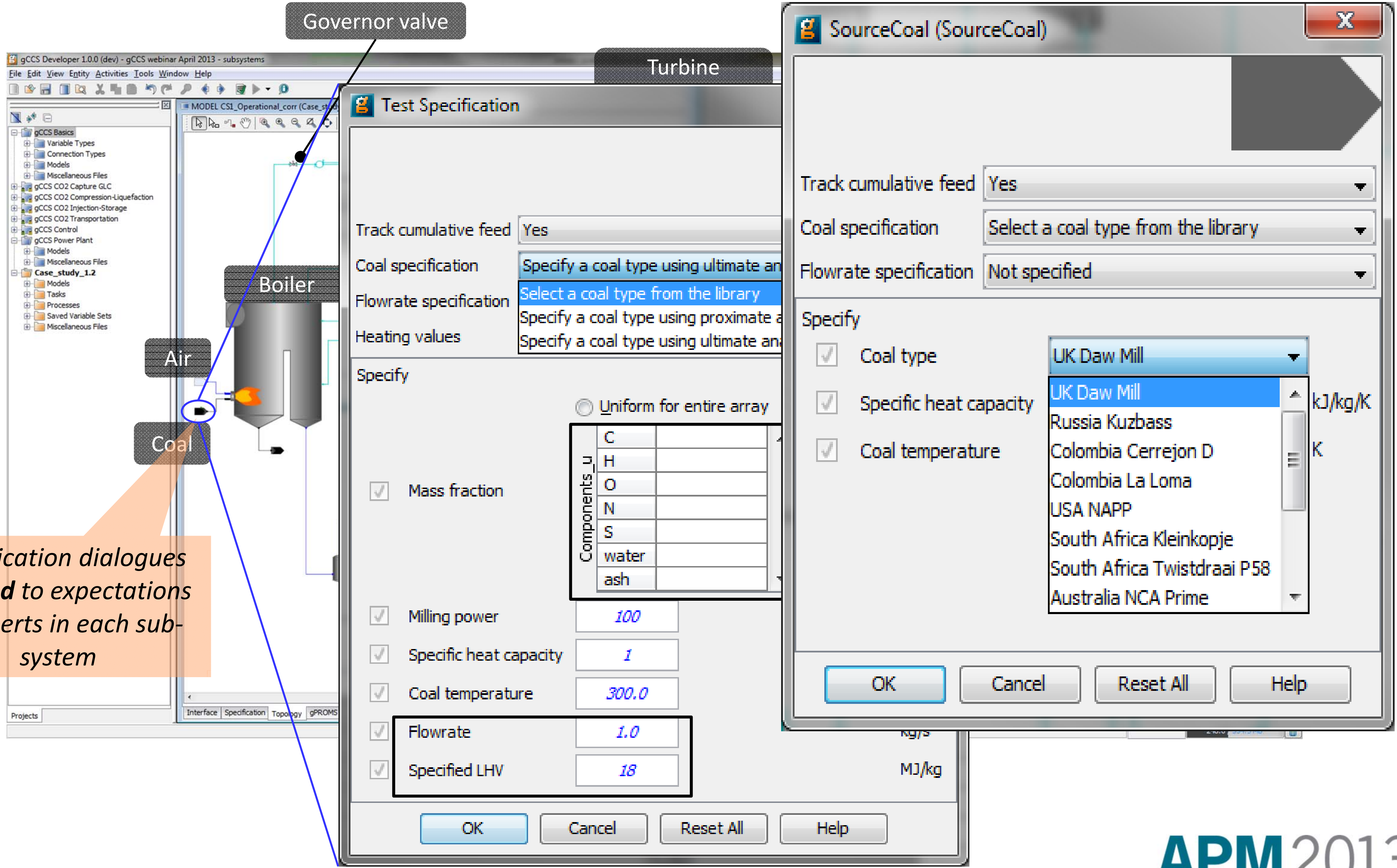
Tool-kit components

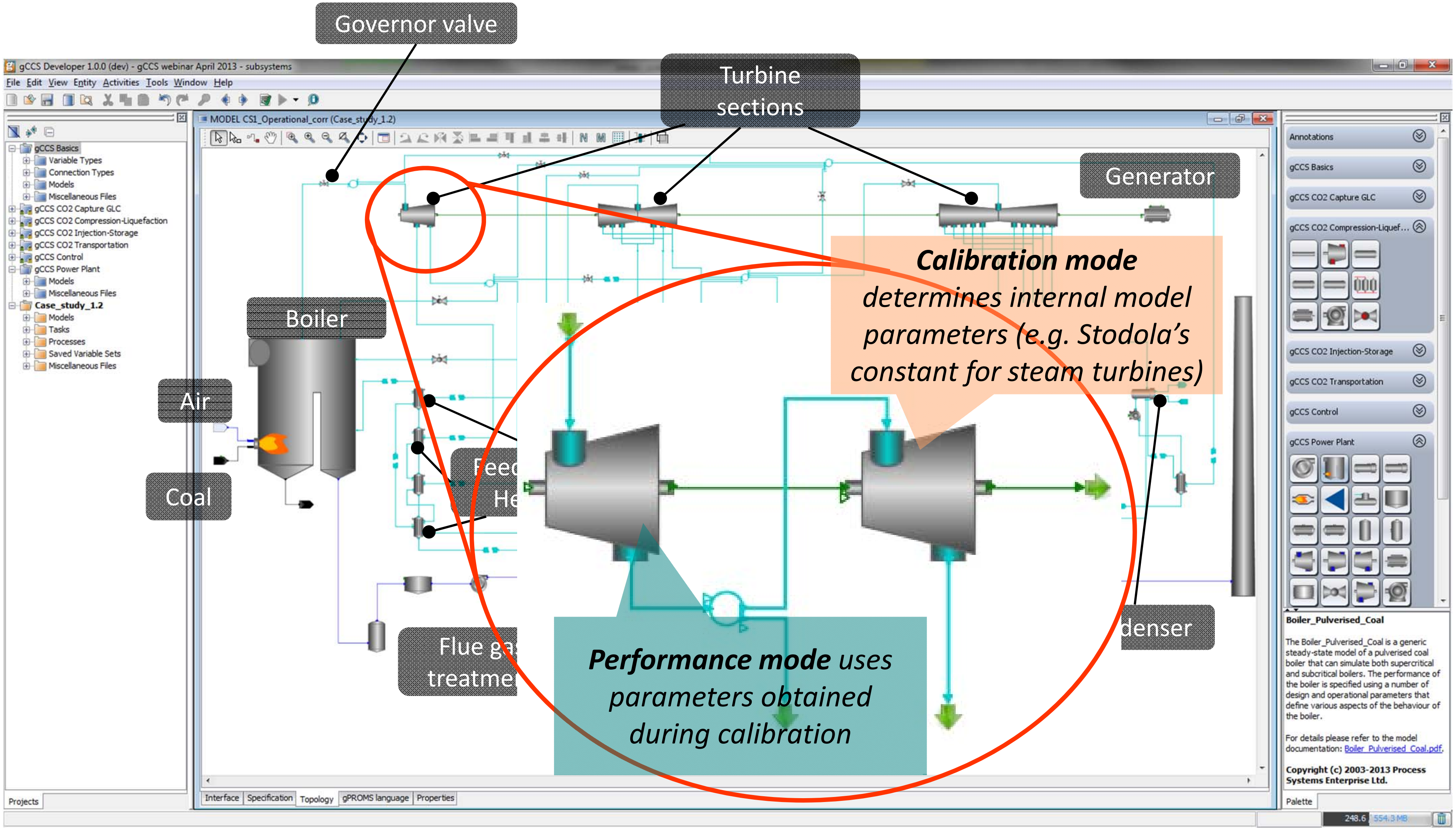
Model libraries – Power plant



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

Tool-kit components

Model libraries – Power plant



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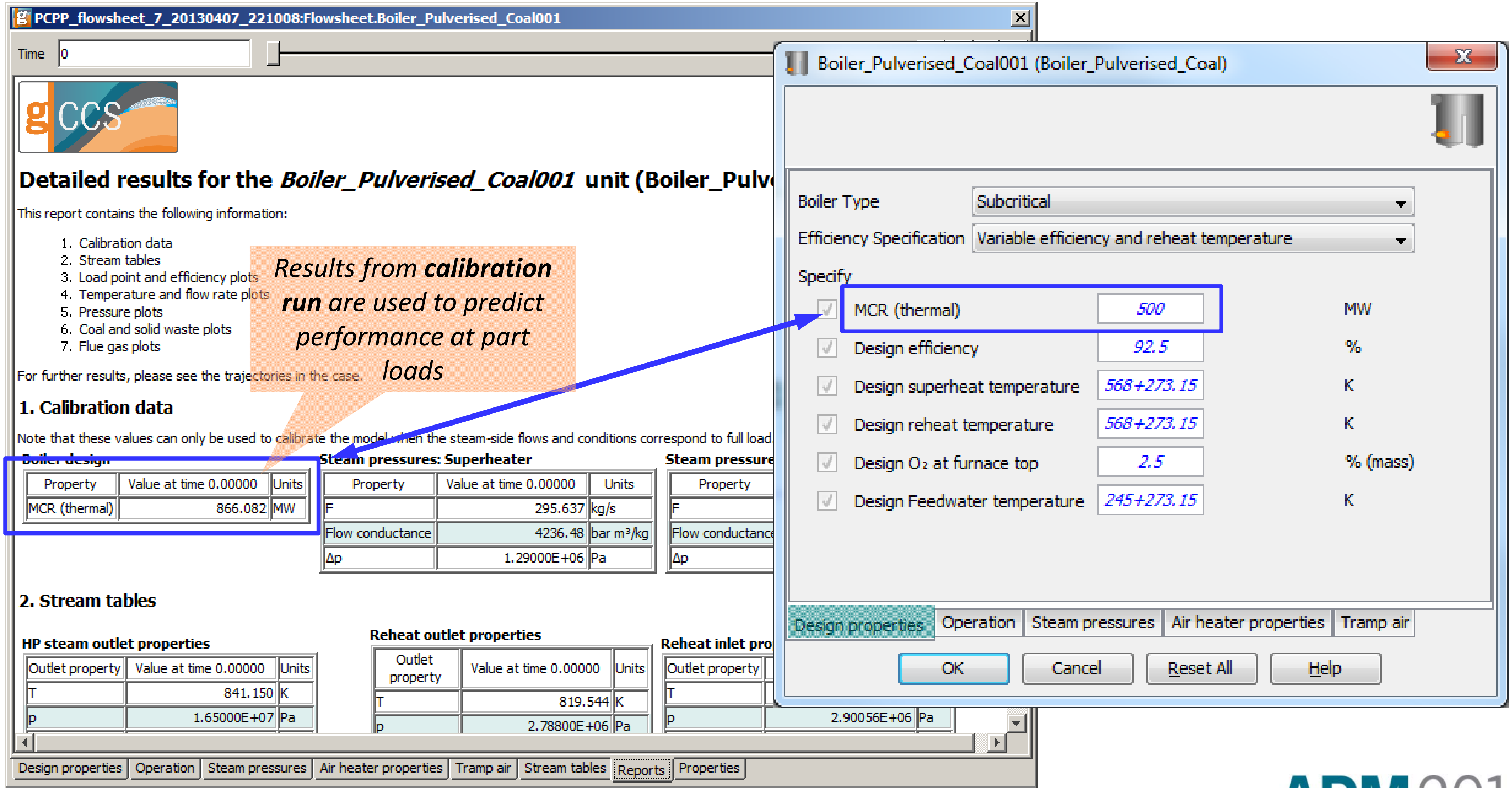
- Calibration vs. performance mode



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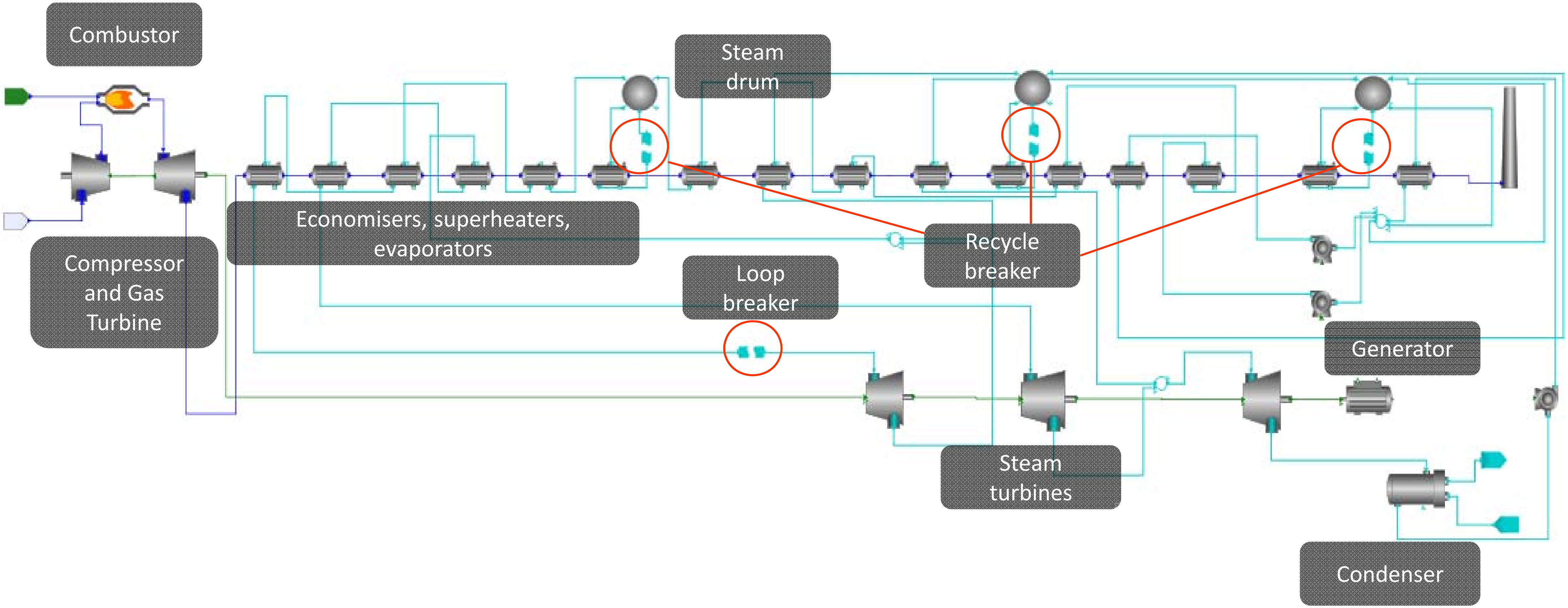
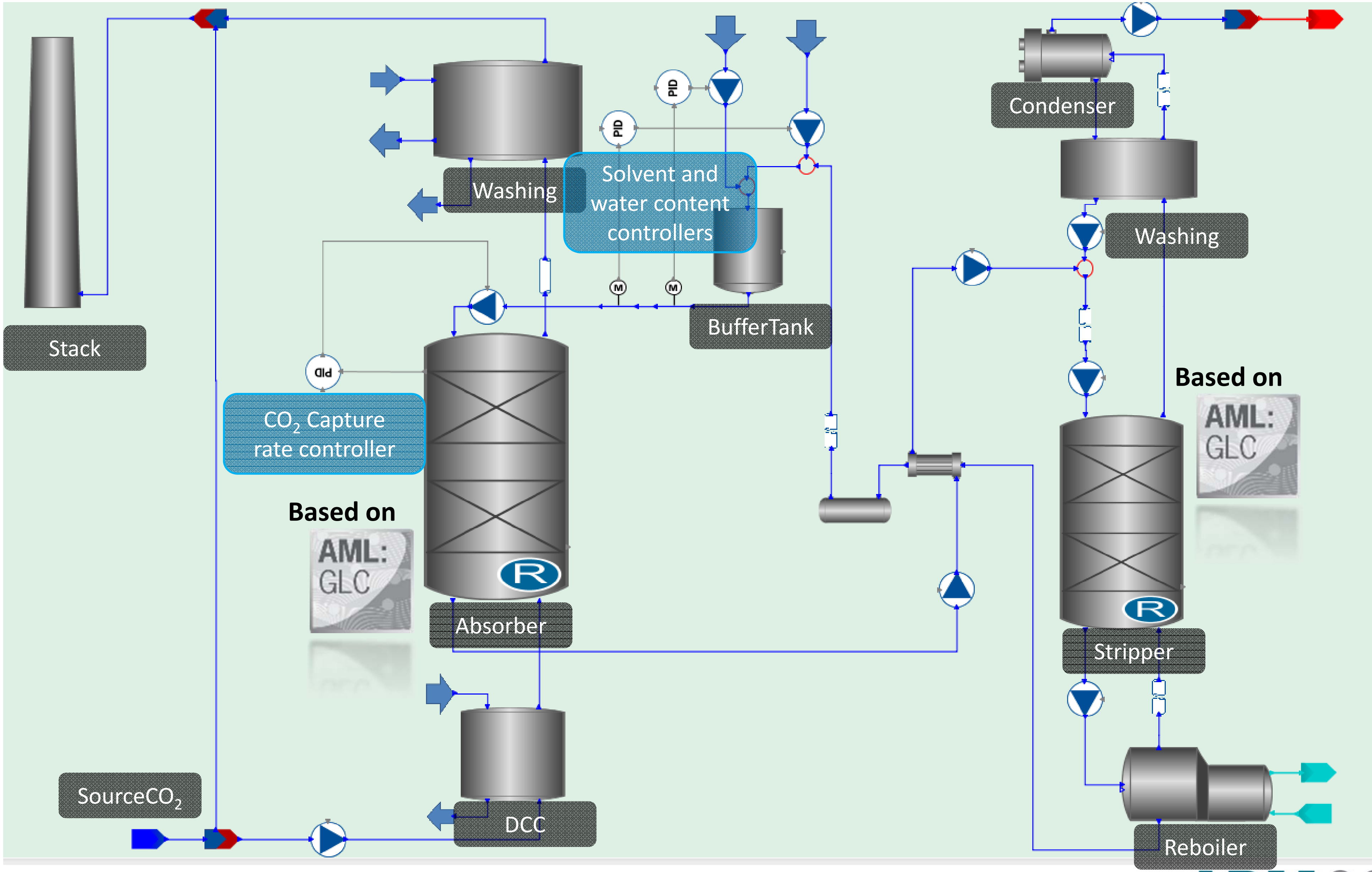
- Combined Cycle Gas Turbine flowsheet



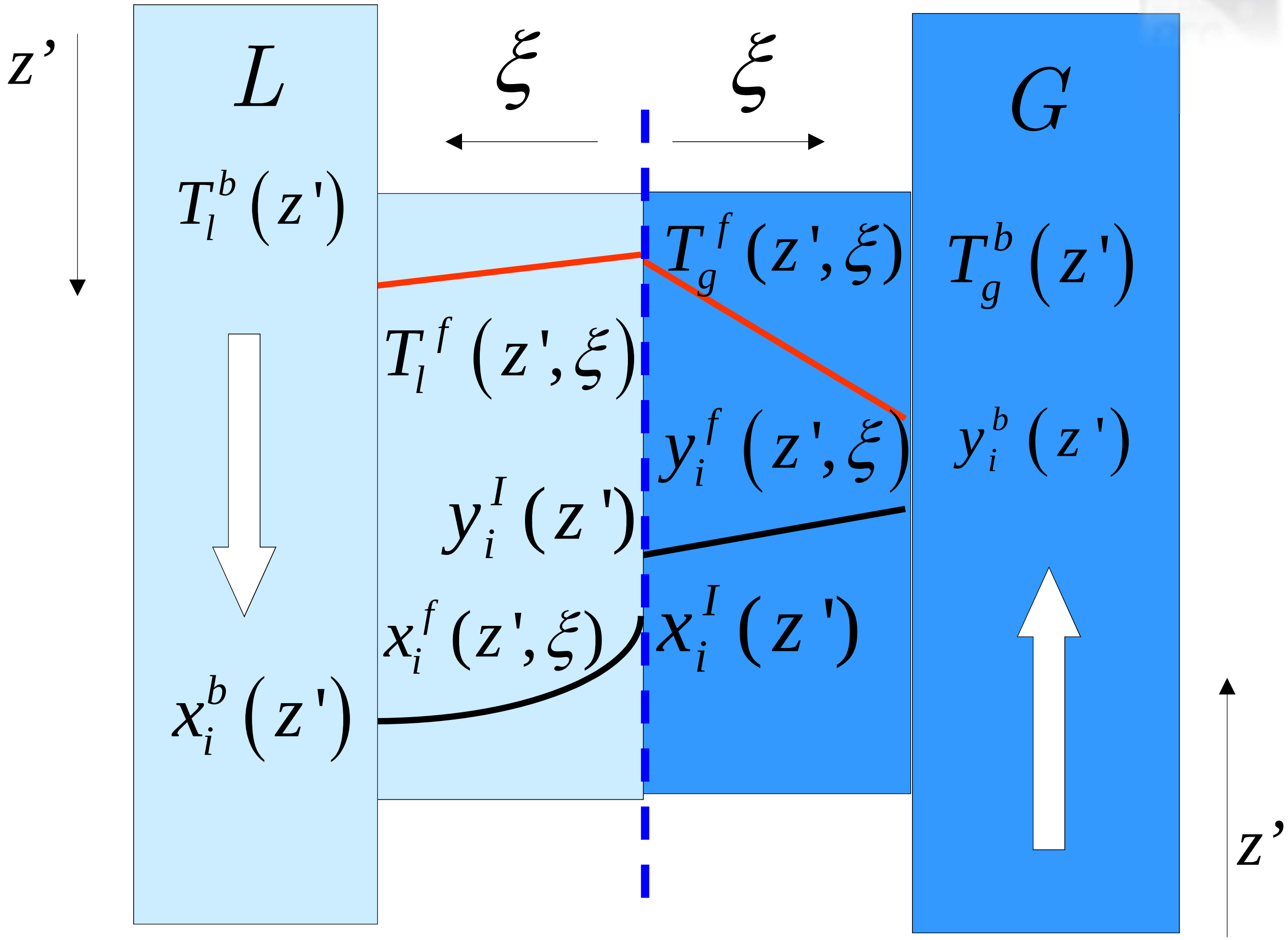
Tool-kit components

Model libraries – CO_2 Capture (chemical and physical absorption)



High-fidelity component models

- Non-equilibrium models
- Models distributed in axial direction and in the direction of the liquid and vapour films
- Energy balance and V/L equilibrium at the interface
- Phase behaviour and chemical equilibrium currently calculated by OLI thermodynamic package
  - to be replaced by gSAFT
- Transport properties
  - Obtained from correlations and Multiflash



Tool-kit components

Model libraries – CO_2 Capture

$H_2O \Leftrightarrow H(+) + OH(-)$

$HCO_3(-) + OH(-) \Leftrightarrow CO_3(-) + H2O$

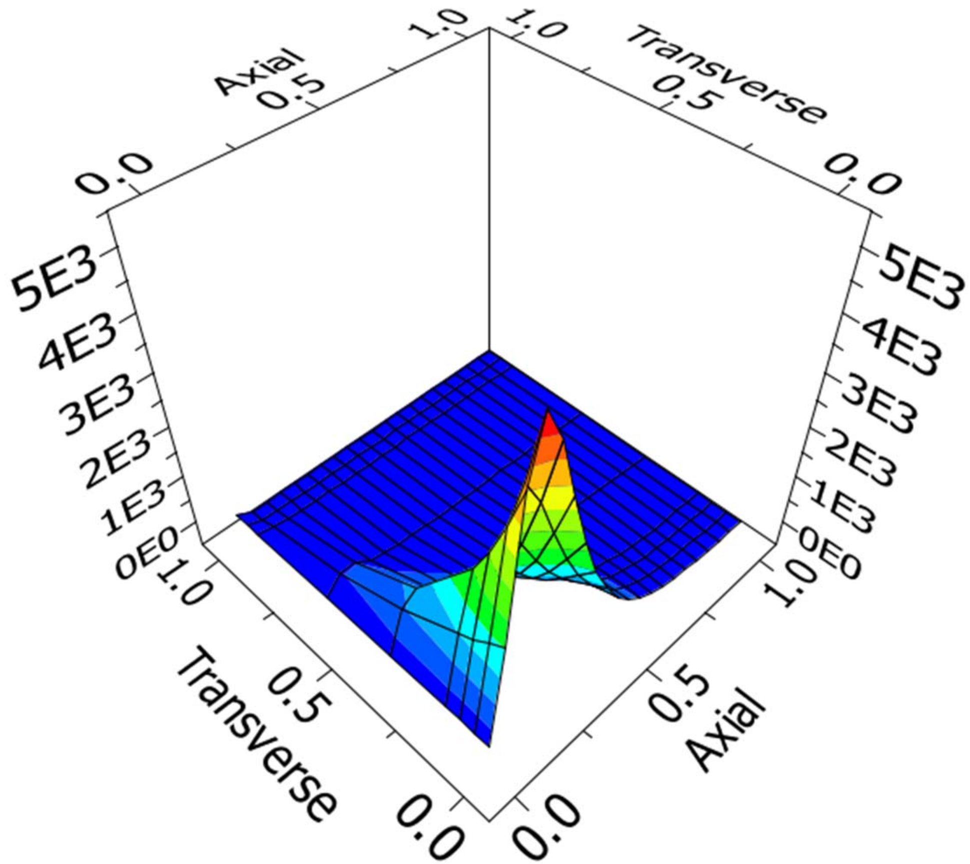
$CO_2 + OH(-) \Leftrightarrow HCO_3(-)$

$\mathbf{CO_2 + MEXH \Leftrightarrow MEXCO_2(-) + H(+)}$

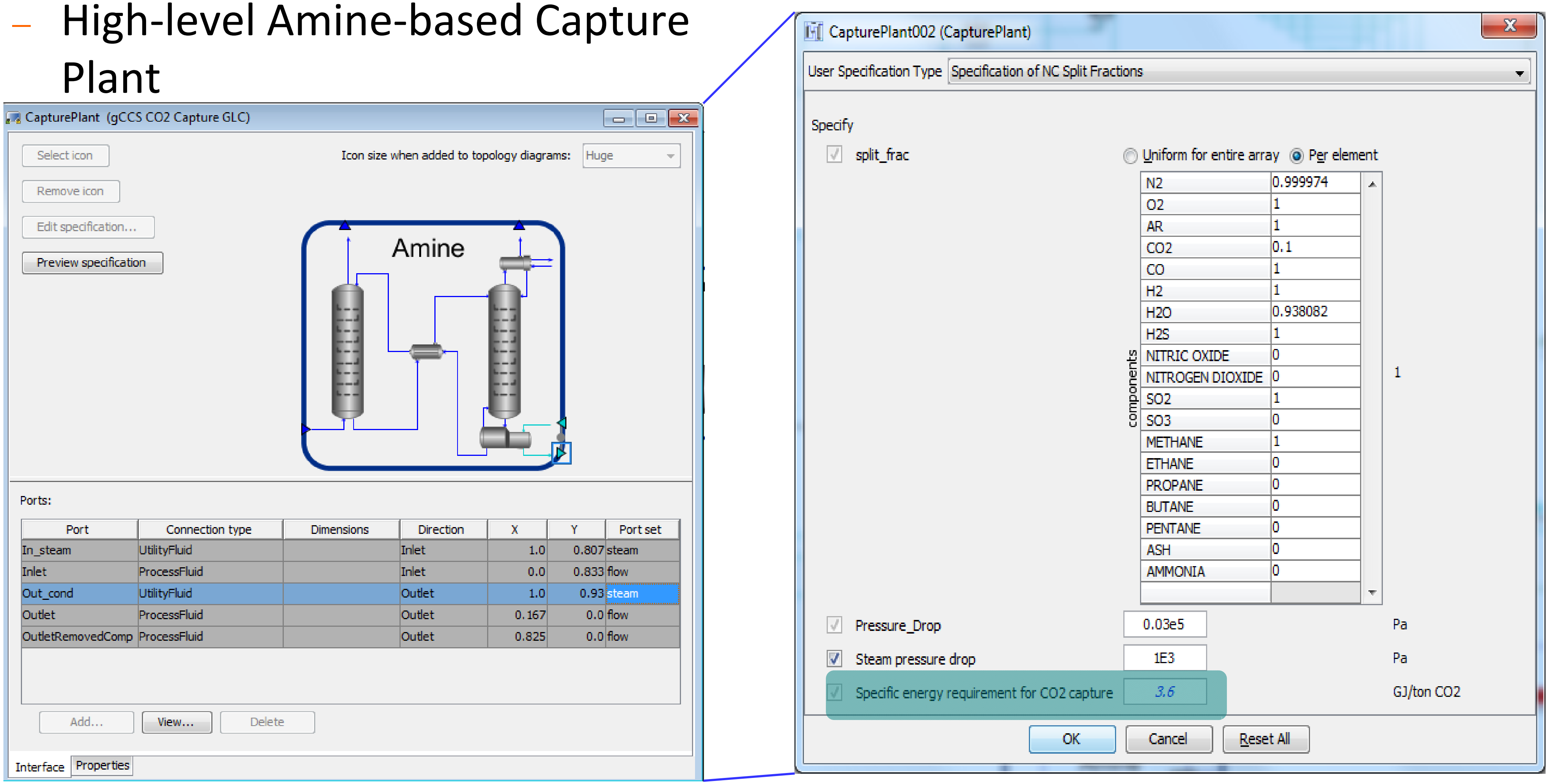
$MEXH + H2O \Leftrightarrow MEXH_2(+) + OH(-)$

Carbamate formation, kinetically controlled reaction

Transversal and axial profiles for the reaction rate of carbamate formation



- Different level of fidelity for systems modelling
  - High-level Amine-based Capture Plant

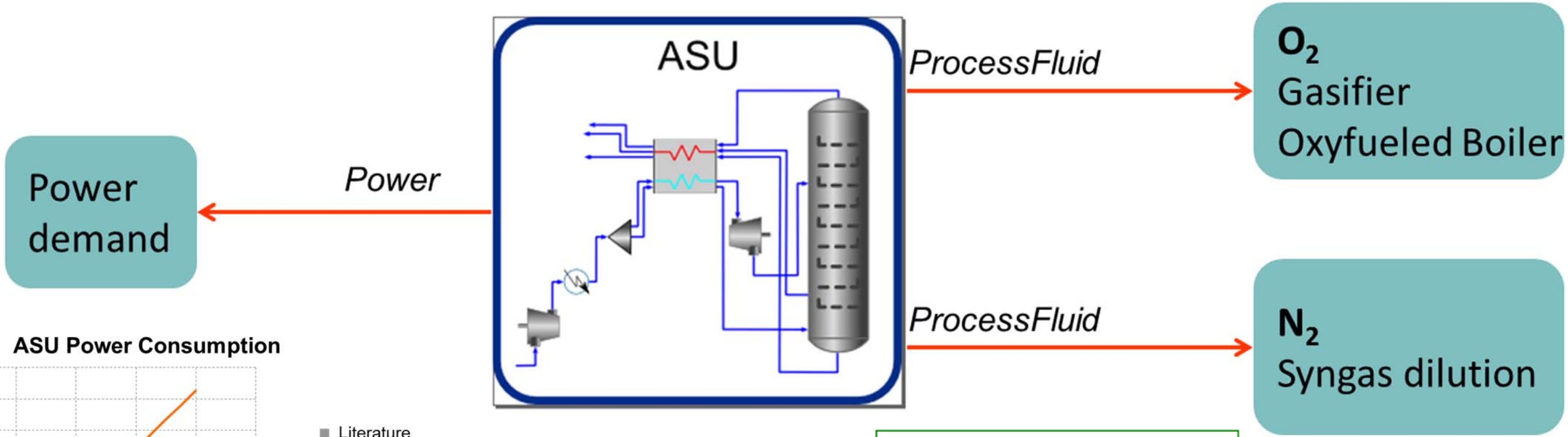


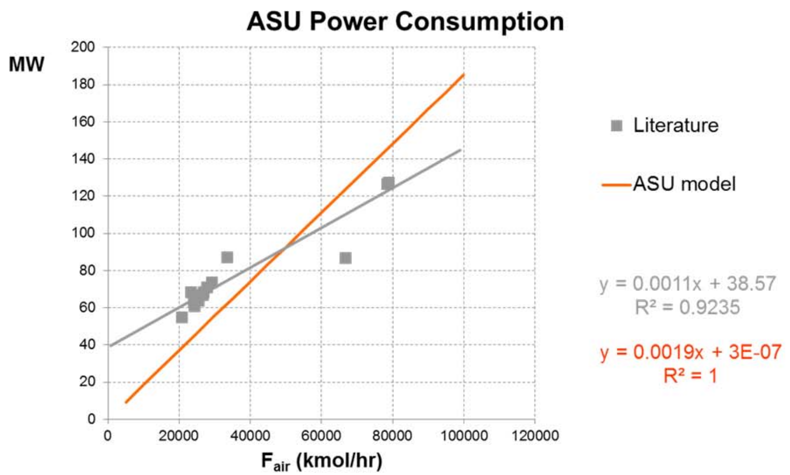
Tool-kit components

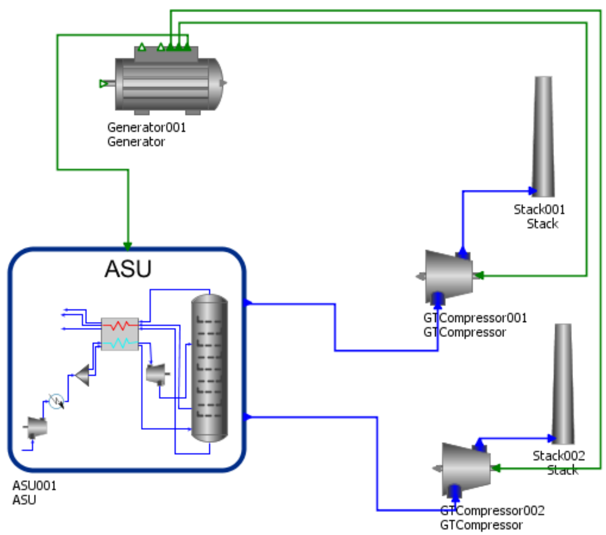
Model libraries – CO_2 Capture (pre-combustion)

- Different level of fidelity for systems modelling
  - High-level Air Separation Unit

Model acts as Source of O_2 and N_2 and calculates power demand



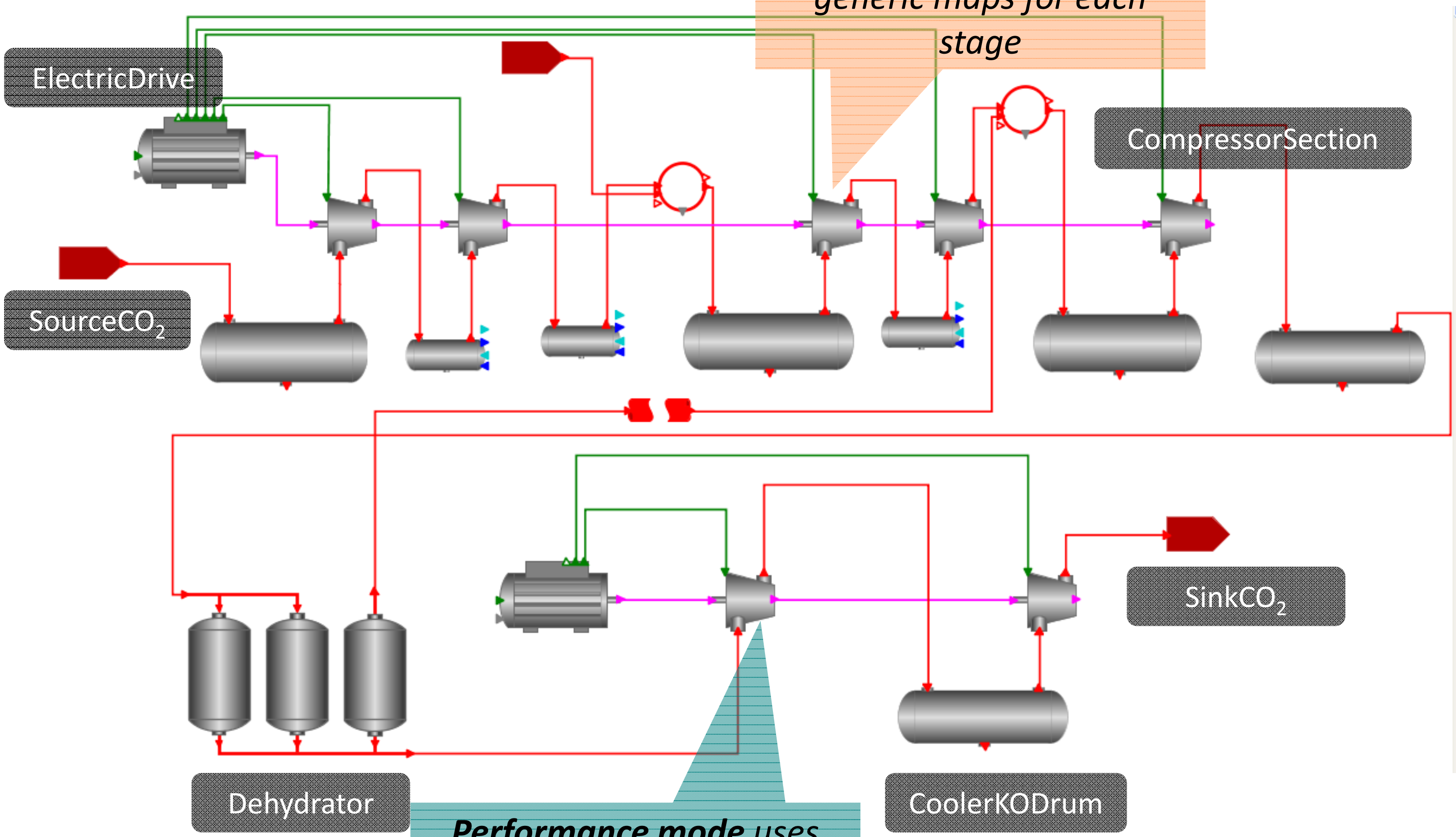




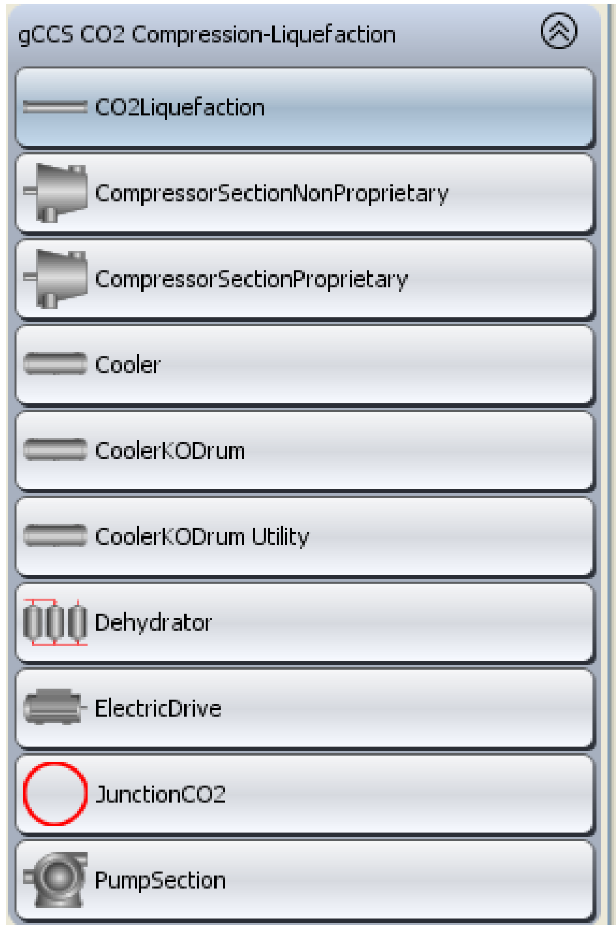
Tool-kit components

Model libraries – CO_2 Compression & Liquefaction

Design mode *determines # of stages and generates generic maps for each stage*



Performance mode *uses user-specified design (# of stages, maps for each stage)*



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- Operational studies – control: Surge avoidance
  - Increase volumetric flowrate in the compressor
    - Recycle compressed flow to the inlet through a recycle loop

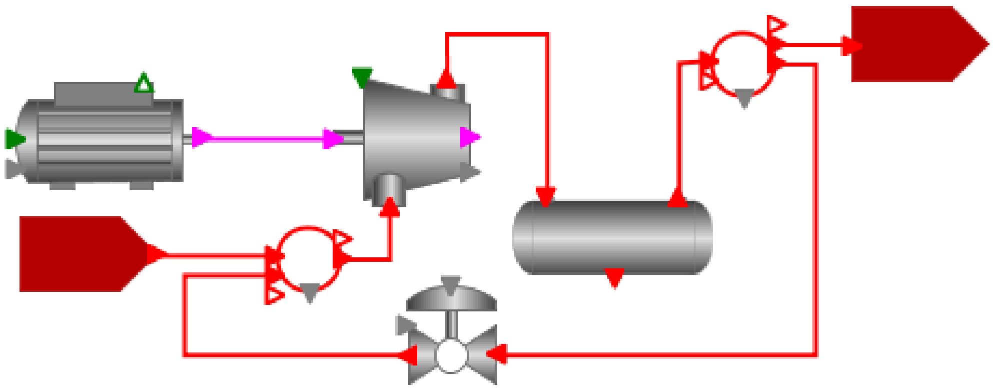


Fig. 4 – Cooled recycle loop used in surge control.

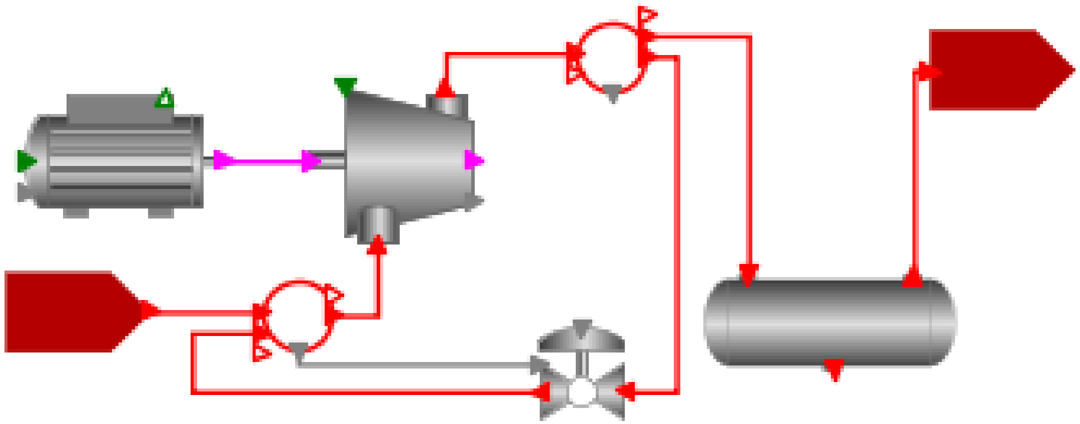
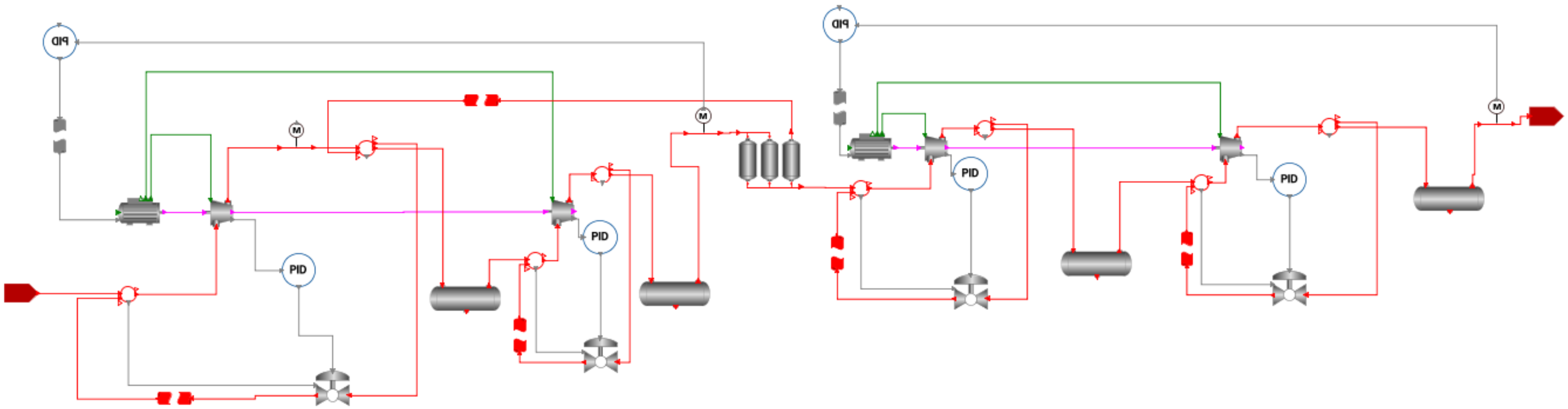
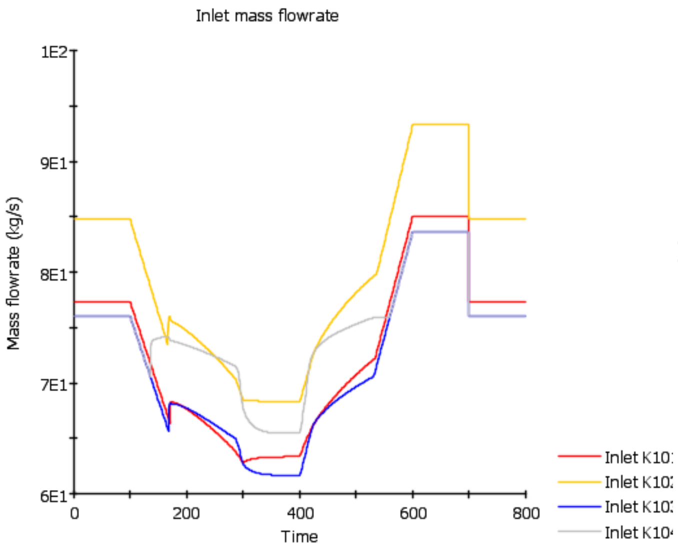


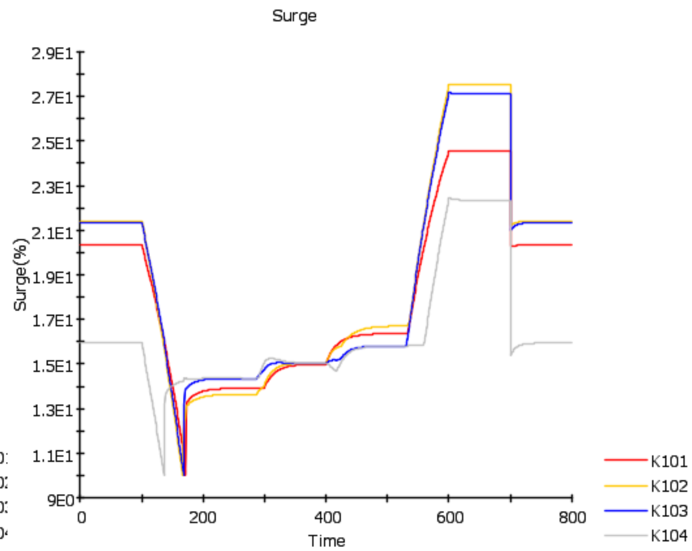
Fig. 5 – Non-cooled recycle loop used in surge control.

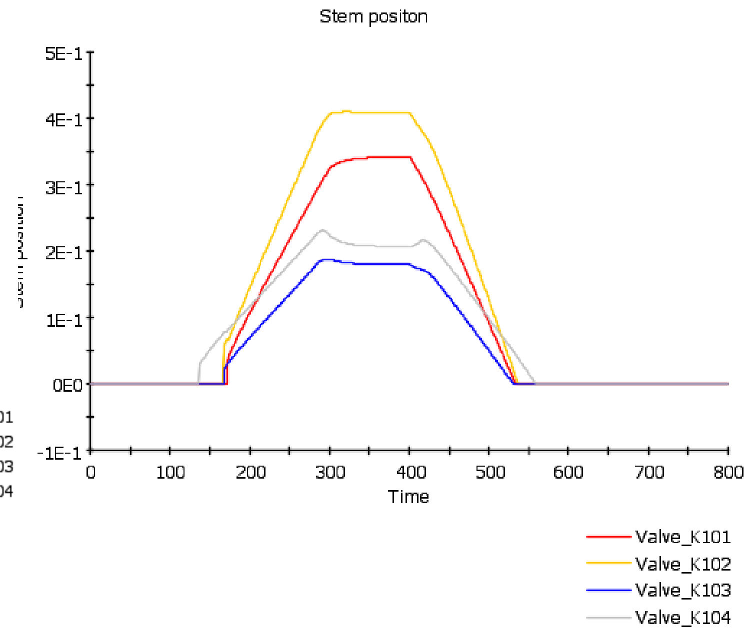
Tool-kit components

Model libraries – CO_2 Compression & Liquefaction





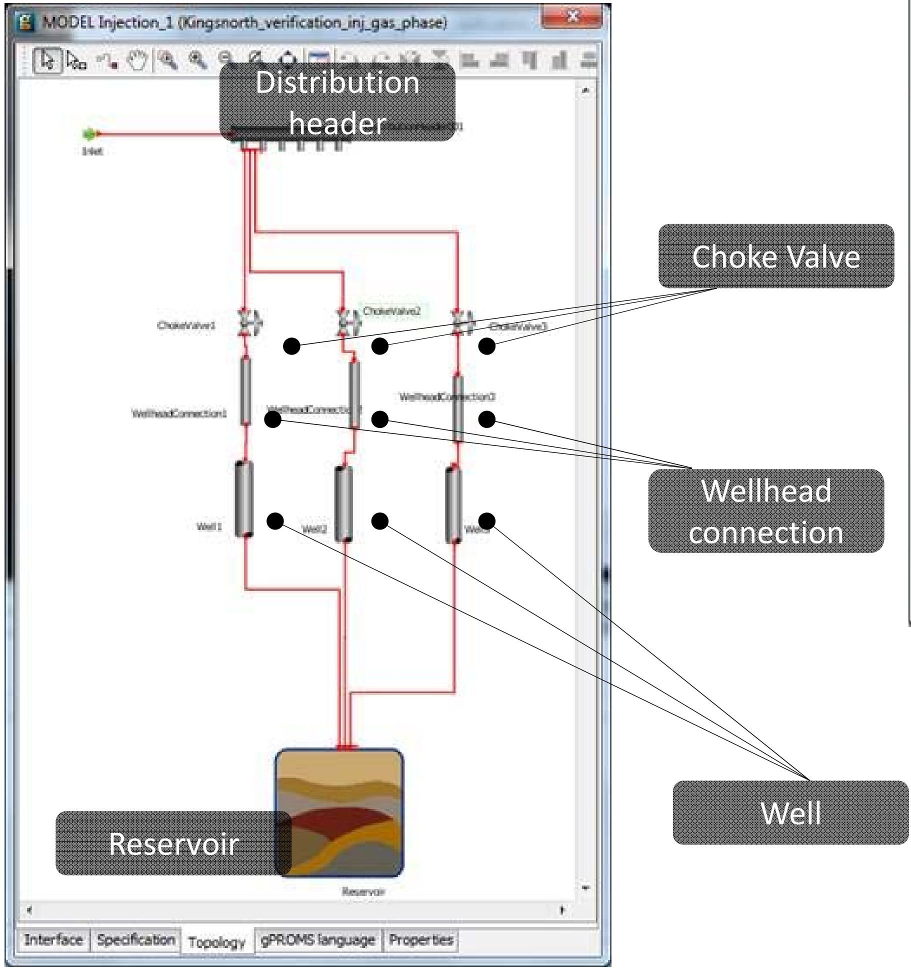


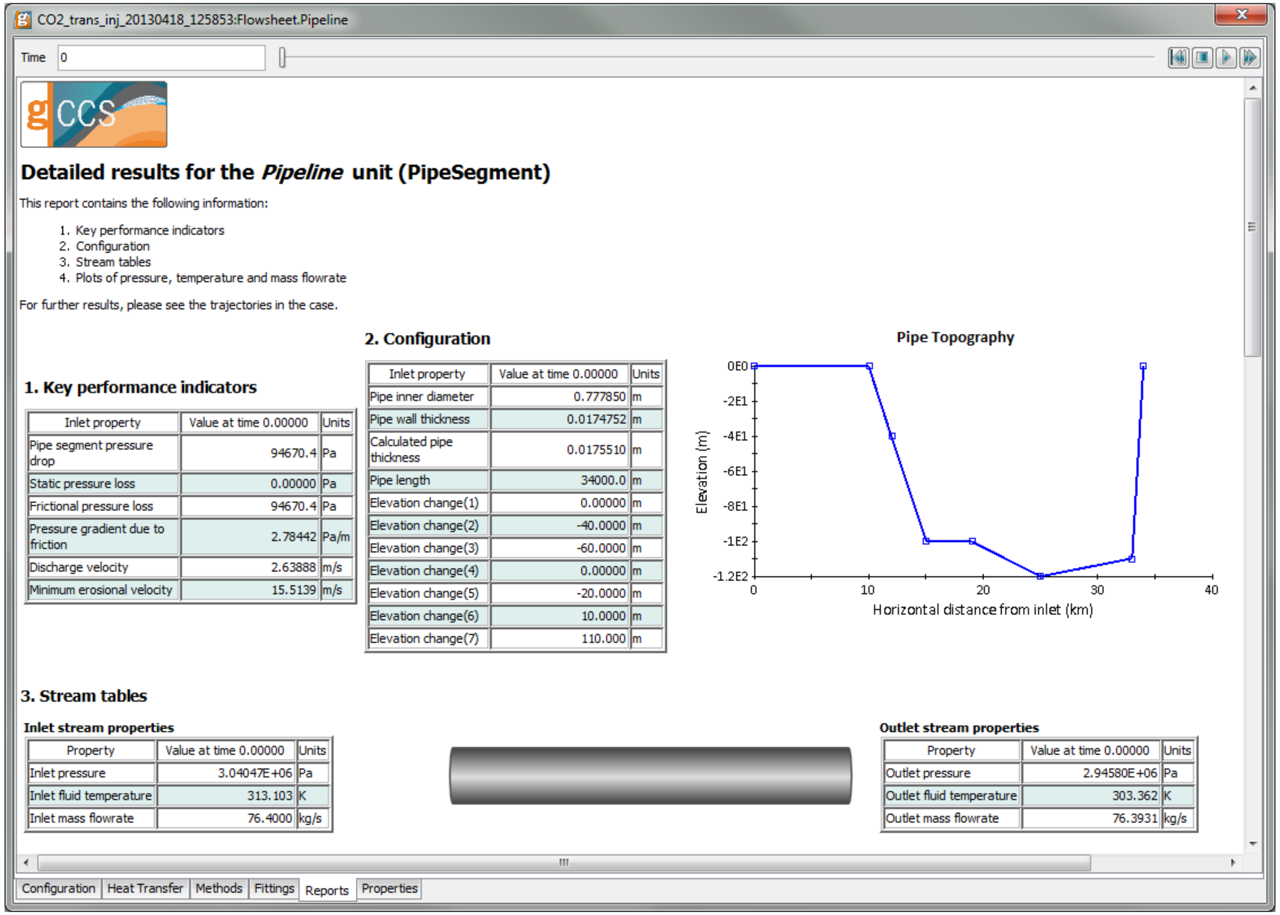


Tool-kit components

Model libraries – CO_2 Transmission and Injection/Storage

Detailed reports




CO2_trans_inj_20130418_125853:Flowsheet.Pipeline

Time 0

gCCS

Detailed results for the *Pipeline* unit (PipeSegment)

This report contains the following information:

1. Key performance indicators
2. Configuration
3. Stream tables
4. Plots of pressure, temperature and mass flowrate

For further results, please see the trajectories in the case.

1. Key performance indicators

Inlet property	Value at time 0.00000	Units
Pipe segment pressure drop	94670.4	Pa
Static pressure loss	0.00000	Pa
Frictional pressure loss	94670.4	Pa
Pressure gradient due to friction	2.78442	Pa/m
Discharge velocity	2.63888	m/s
Minimum erosional velocity	15.5139	m/s

2. Configuration

Inlet property	Value at time 0.00000	Units
Pipe inner diameter	0.777850	m
Pipe wall thickness	0.0174752	m
Calculated pipe thickness	0.0175510	m
Pipe length	34000.0	m
Elevation change(1)	0.00000	m
Elevation change(2)	-40.0000	m
Elevation change(3)	-60.0000	m
Elevation change(4)	0.00000	m
Elevation change(5)	-20.0000	m
Elevation change(6)	10.0000	m
Elevation change(7)	110.000	m

3. Stream tables

Inlet stream properties

Property	Value at time 0.00000	Units
Inlet pressure	3.04047E+06	Pa
Inlet fluid temperature	313.103	K
Inlet mass flowrate	76.4000	kg/s

Outlet stream properties

Property	Value at time 0.00000	Units
Outlet pressure	2.94580E+06	Pa
Outlet fluid temperature	303.362	K
Outlet mass flowrate	76.3931	kg/s

Configuration | Heat Transfer | Methods | Fittings | Reports | Properties

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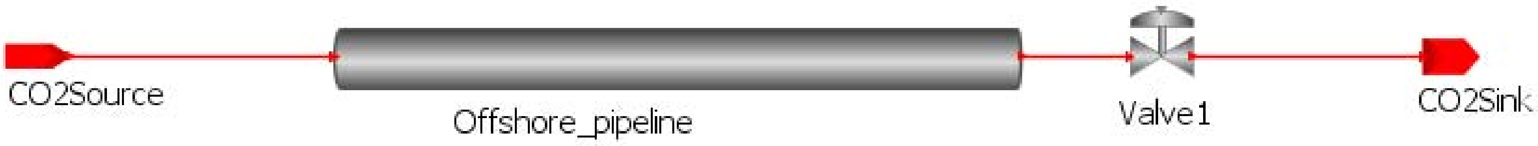
Tool-kit components

Model libraries – CO_2 Transmission and Injection/Storage

System dynamics

– Simulating **line-packing operation**: Sudden valve closure

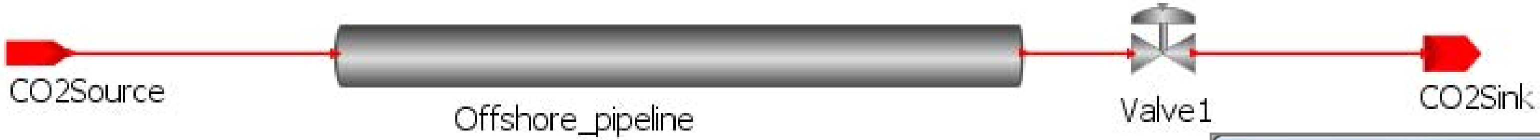


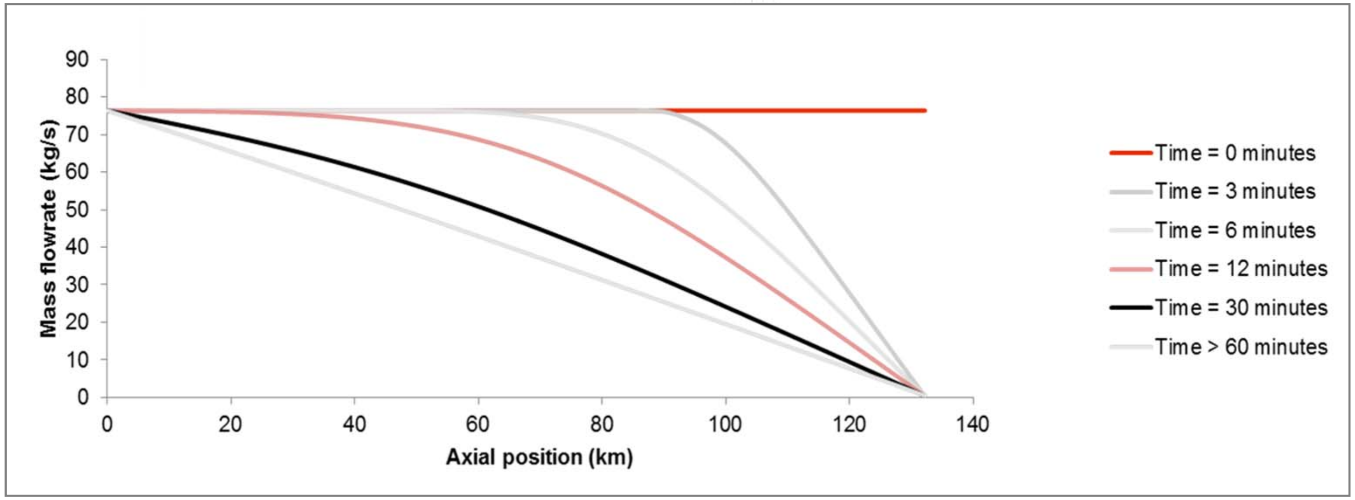
- Assumed constant inlet flowrate at CO2Source (275tonnes CO_2 per day)
- Gas phase injection with discharge pressure in CO2 sink ~ 21bara
- Total pipeline length – 132.2km
- Pipeline is located offshore (in water)

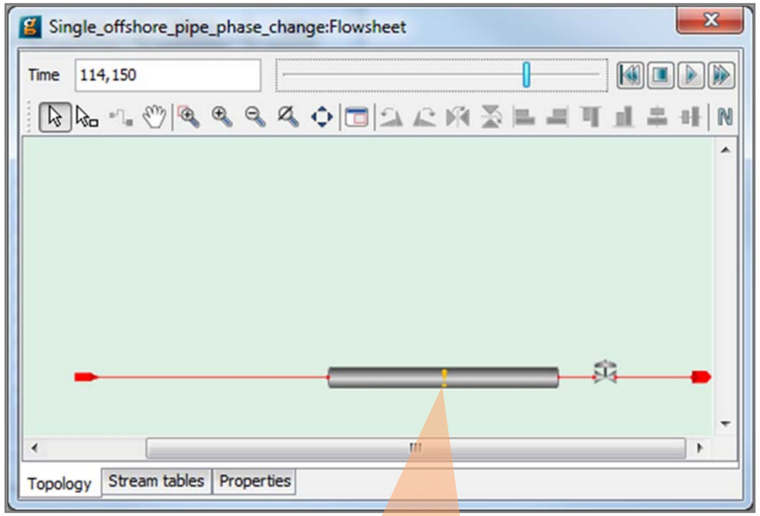
Tool-kit components

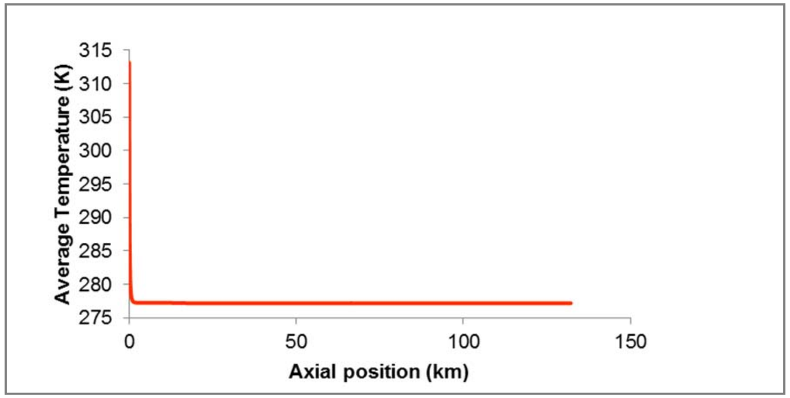
Model libraries – CO_2 Transmission and Injection/Storage

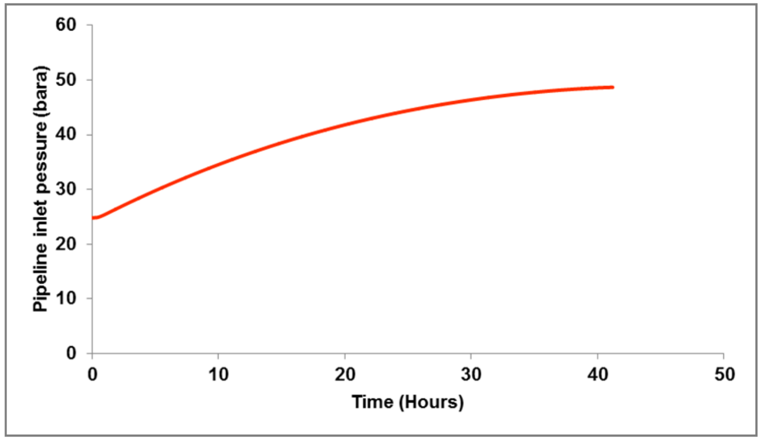
- System dynamics
  - Simulating **line-packing operation**: Sudden valve closure











***Warning**: Phase change identified!*

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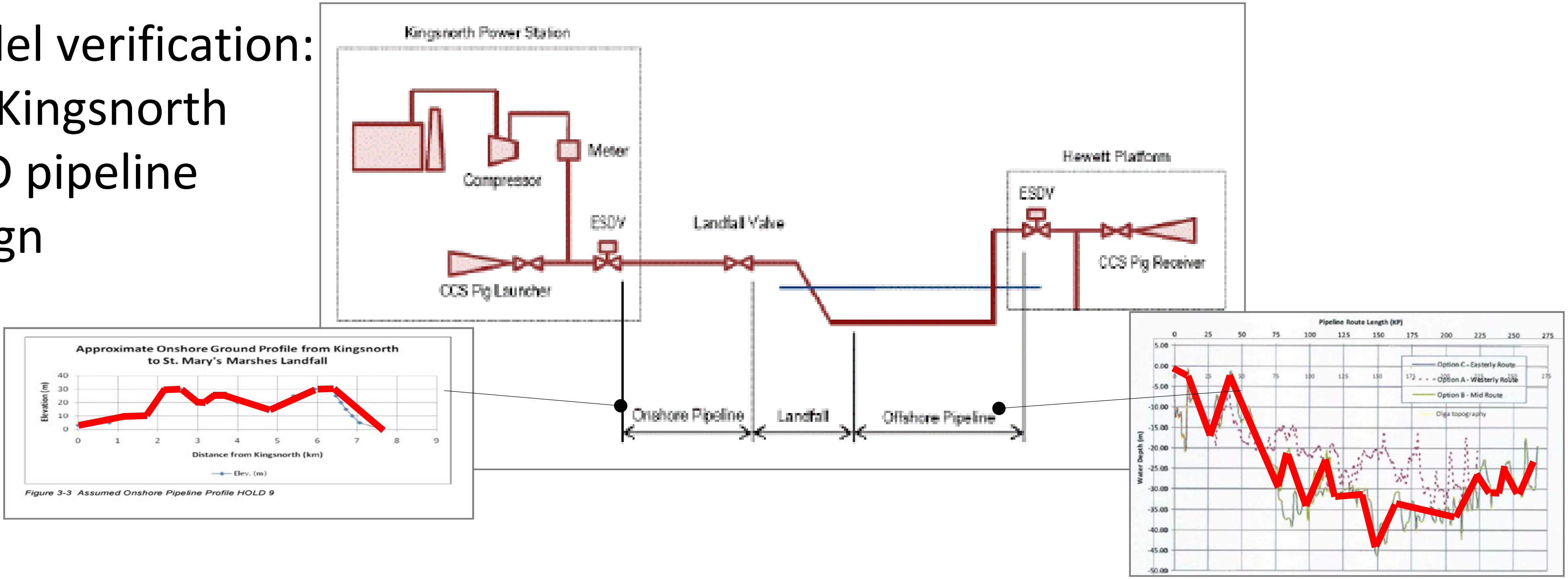
Tool-kit components

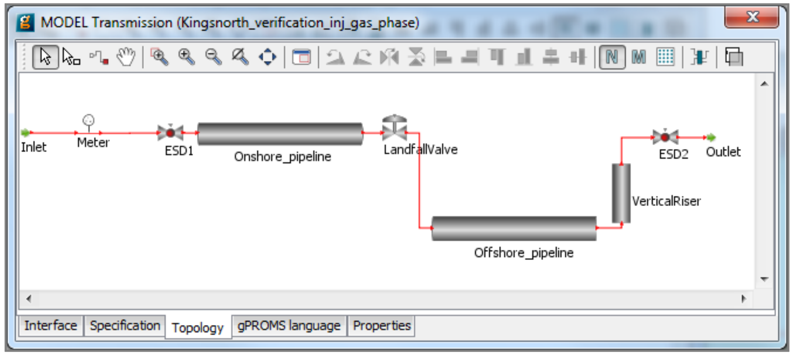
Model libraries – CO_2 Transmission and Injection/Storage

Model verification: e.g. Kingsnorth FEED pipeline design



	Kingsnorth pipeline ΔP (bar)	gCCS pipeline ΔP	% Error
Dense phase	7.6	7.18	5.59
Gas phase	5.6	5.31	5.18

	Kingsnorth fluid temperature at top of riser (K)	gCCS fluid temperature at top of riser (K)	Absolute error in T (K) at top of riser
Dense phase	3.6	4.47	0.87
Gas phase	3.0	3.27	0.27



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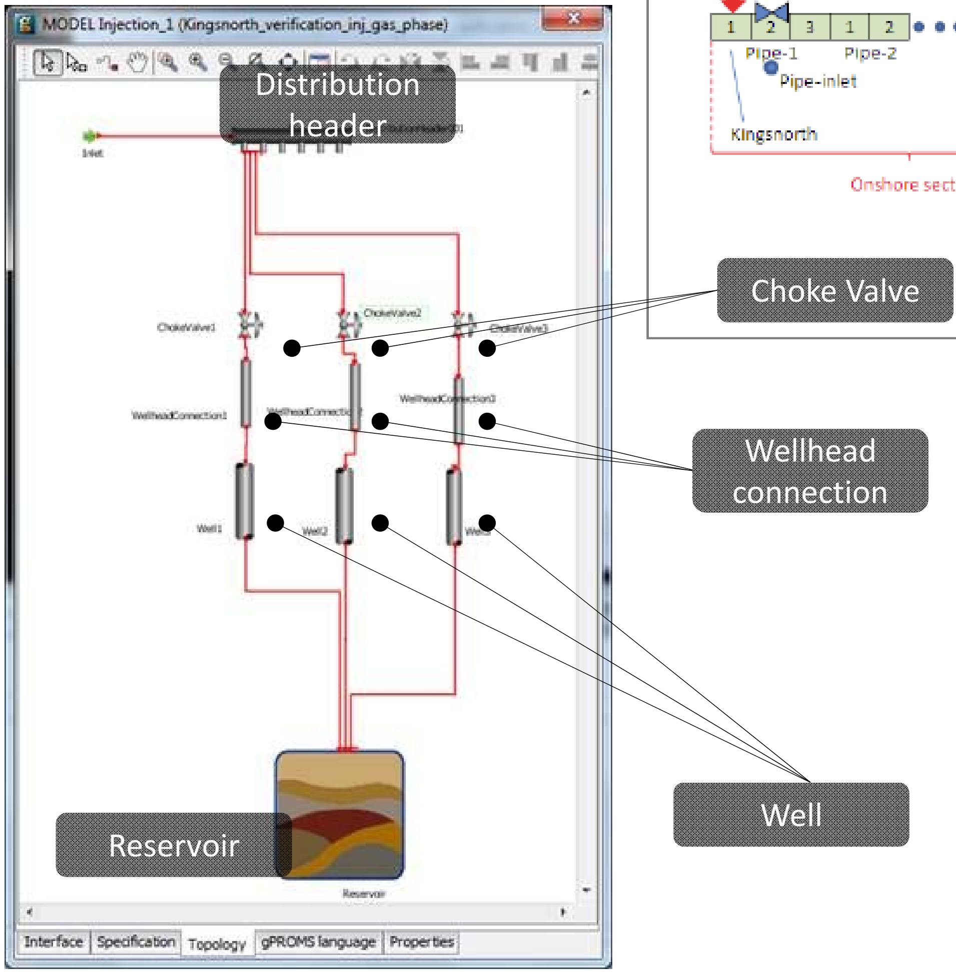
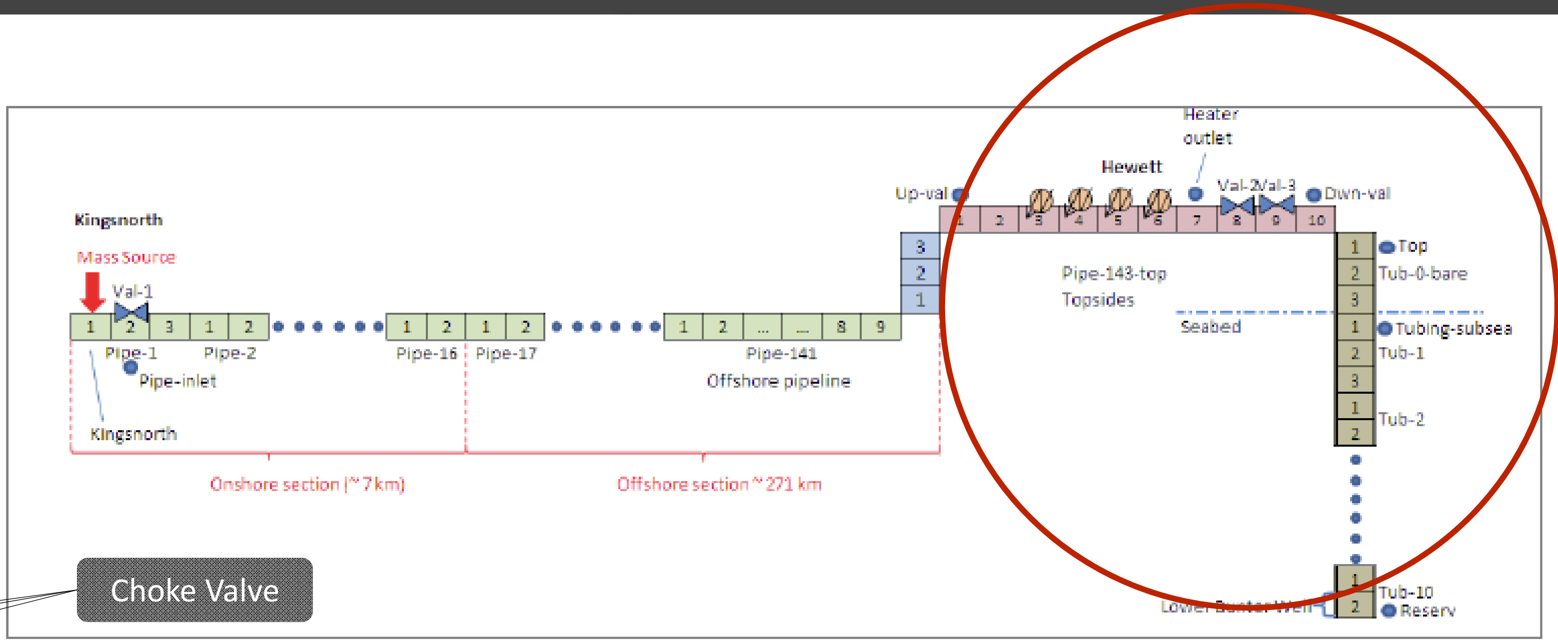
Tool-kit components

Model libraries – CO_2 Transmission and Injection/Storage

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





For gas phase operation (reservoir pressure 2.1barg)	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

Tool-kit components

Physical properties

- Different material/species within the same sub-system
  - e.g. in power plant: coal, water, flue gas
- Different materials/species in different sub-systems
  - e.g. MEA in CO_2 capture plant
- Need different thermodynamic models for different materials, e.g.
  - cubic EoS (PR 78) for flue gas in power plant
  - Corresponding States (Steam Tables) for pure water

  gPROMS Properties (Multiflash®)

  - SAFT for amine-containing streams in CO_2 capture
  - SAFT for near-pure post-capture CO_2 streams

  gSAFT
- Transport properties obtained from gPROMS Properties
  - models/ correlations

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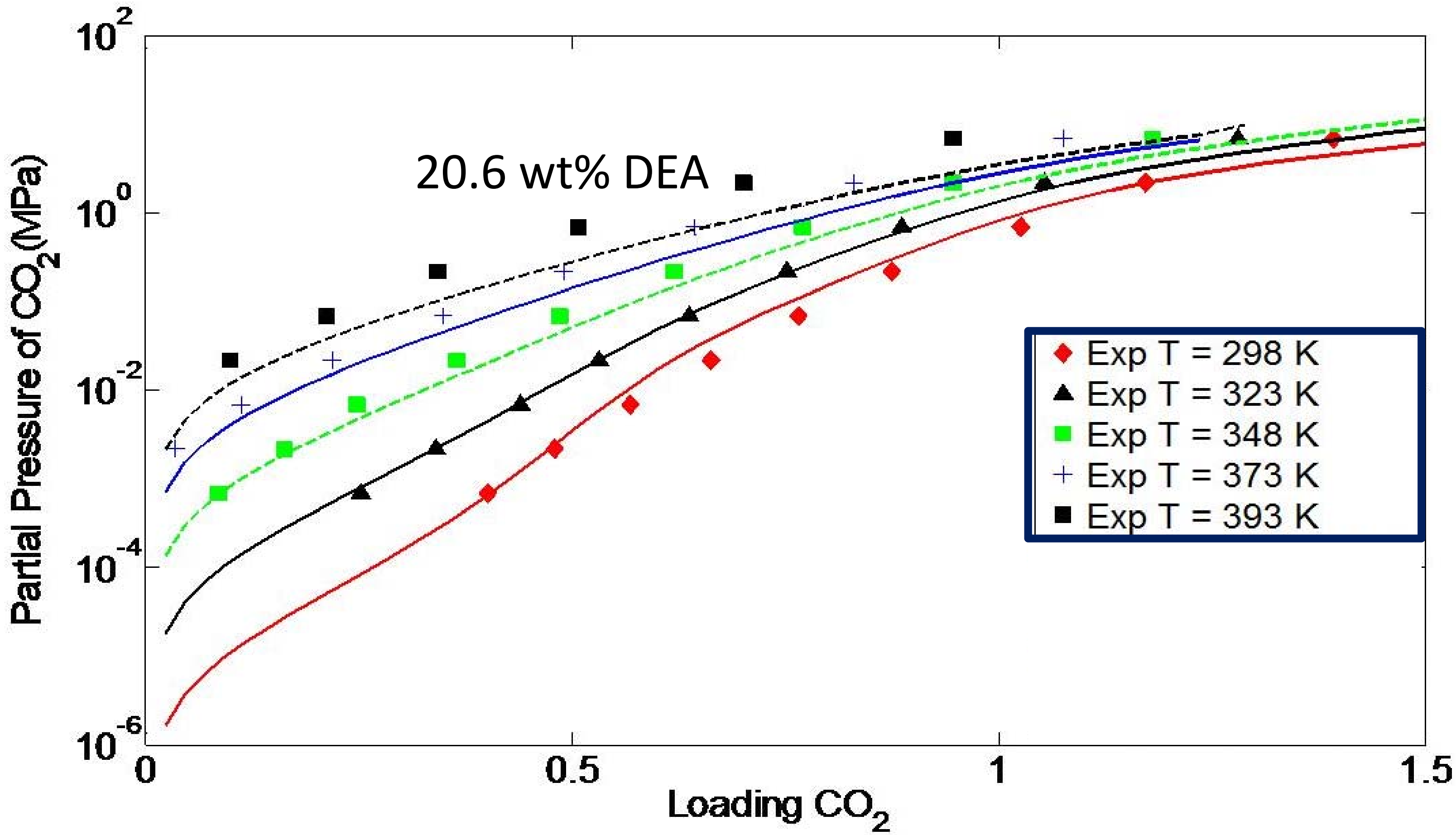
Why gSAFT?

Accurate physical property predictions for CO_2 absorption

Ternary mixture of diethanolamine (DEA) + H_2O+ CO_2



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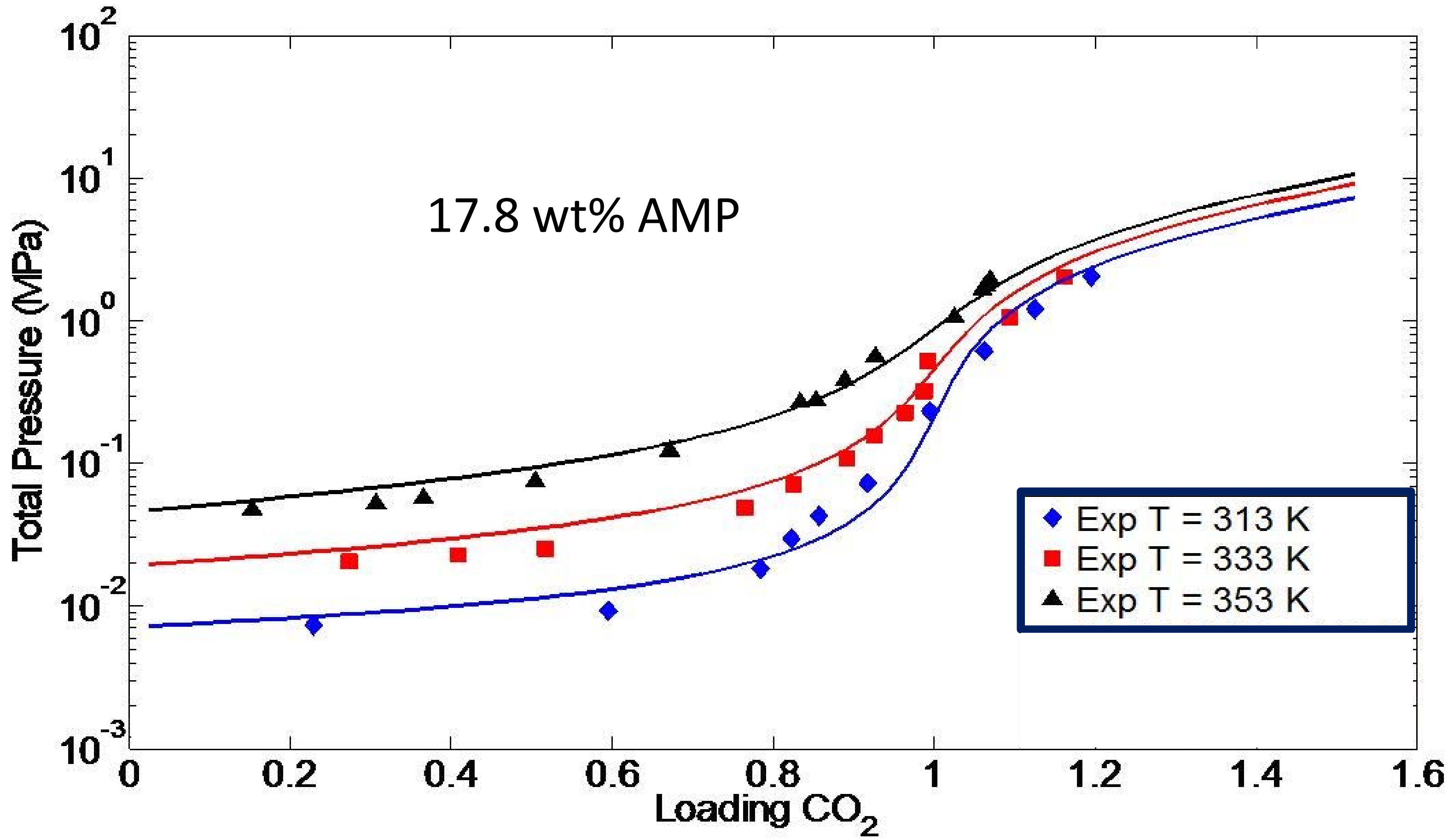
Why gSAFT?

Accurate physical property predictions for CO_2 absorption

Ternary mixture of 2-amino-2-methyl-1-propanol (AMP) + H_2O+ CO_2



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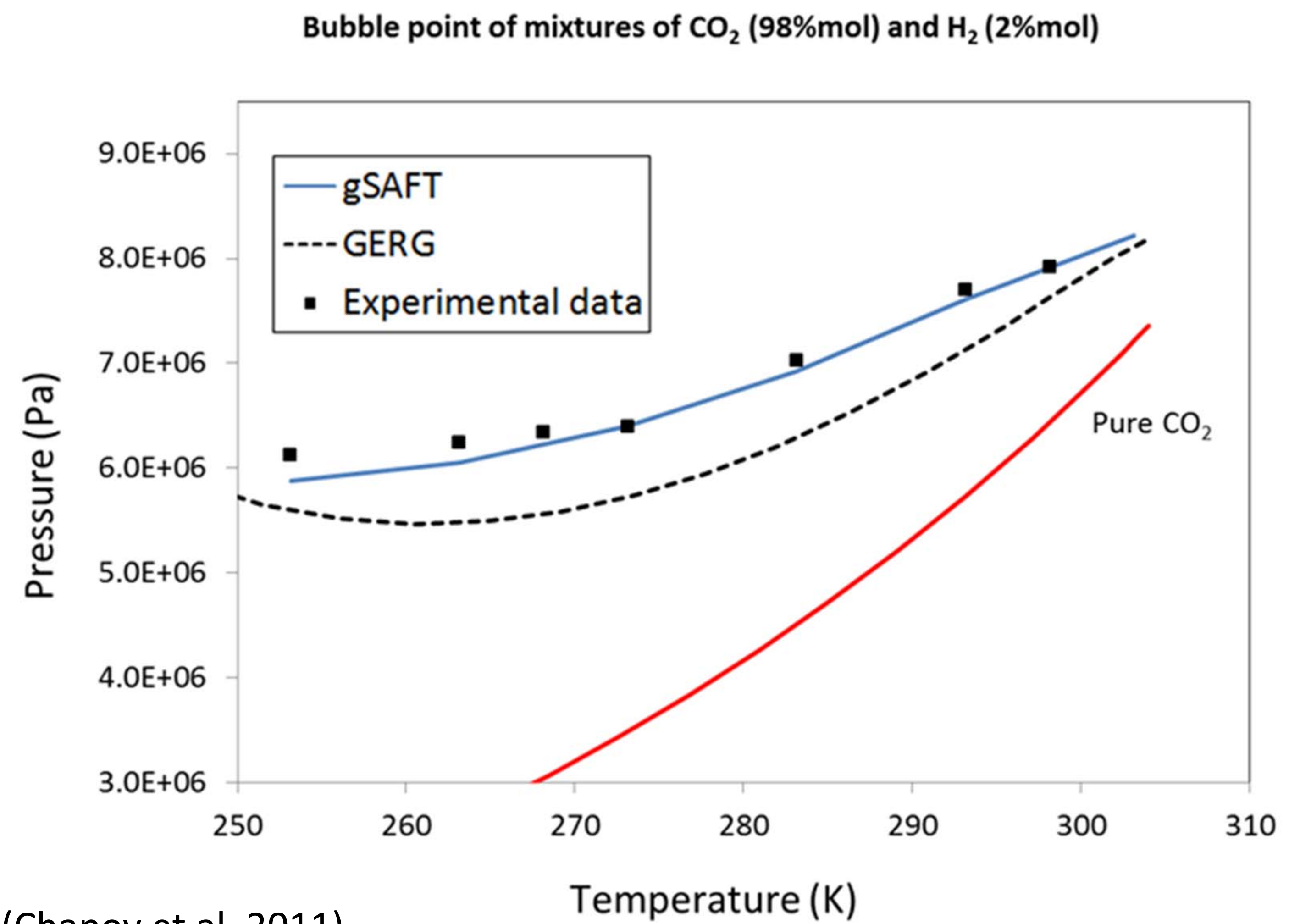
Why gSAFT?

Accurate prediction of phase envelope for near-pure CO_2 mixtures



(Chapoy et al, 2011)

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Tool-kit components

Interfaces to 3rd party modelling tools

- Direct interfacing / co-simulation – based on gPROMS's Foreign Object (FO) interface
  - Steady-state modelling and simulation packages (E.ON's PROATES)
  - Equipment design tools (Rolls-Royce's CompPerform/CompSelect)

- Model fitting
  - Incorporate reduced-order models of high-fidelity equipment models

Summary

What is gCCS?

- A system-wide gPROMS-based modelling platform for “full” CCS chains
  - Build and validate models
  - Simulate CCS systems from source to sink within a single environment
  - Optimise entire CCS chains or parts thereof
- … with pre-installed components for
  - Conventional (coal-fired, CCGT) and non-conventional (oxy-fuel, IGCC) power generation
  - Solvent-based CO_2 capture (both chemical and physical processes)
  - Compression & Liquefaction
  - Transportation (on- and off-shore pipelines)
  - Injection in sub-sea storage
  - State-of-the-art physical properties models for the mixtures along the CCS chain
- … considering various levels of complexity

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When?

- **Now**
  - Conventional power (PC, CCGT), capture (chemical absorption), compression & transportation/injection models
  - Full chain simulation demonstrated
  - gCCS v1.0 alpha available for evaluation to selected
    - universities & research consortia
    - lead users among industrial partners
  - Interfaces to 3rd-party models
- **Soon** (3-6 month timescale)
  - IGCC, oxyfuel power generation
  - Capture – physical absorption
  - Integration with advanced physical properties engine (SAFT-γ Mie)
- **To follow** (9 month – 1-year timescale)
  - Costing
  - Project-ready environment

PSE products

The gPROMS product family

gCCS

The gPROMS platform
Unified modelling platform across all products

gPROMS

Model Builder

AML: FBCR | AML: GLC | AML: ADS | AML: MEM

gSOLIDS | gCRYSTAL | gFLARE | gFUELCELL | gCCS

General-purpose Advanced Process Modelling
Powerful custom modelling in a flowsheeting environment

Advanced Model Libraries
World-leading models for reaction & separation

gPROMS platform products
Domain-specific tools for specialists

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Thank you!

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The Advanced Process Modelling Forum