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*The Advanced Process Modeling Forum*

5 - 6 June 2013, New York

# gCCS – whole-chain CCS system modelling

## Enabling technology to accelerate commercialisation and manage technology risk

Alfredo Ramos – Head of CCS & Power Business

PSE

gCCS

A gPROMS PLATFORM PRODUCT

# Overview

- CCS System Modelling Tool-kit project
  - Motivation
  - Aim
- gCCS overview
  - Model libraries
  - Physical properties
  - Interfaces
- Summary

# Motivation for systems modelling for CCS

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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

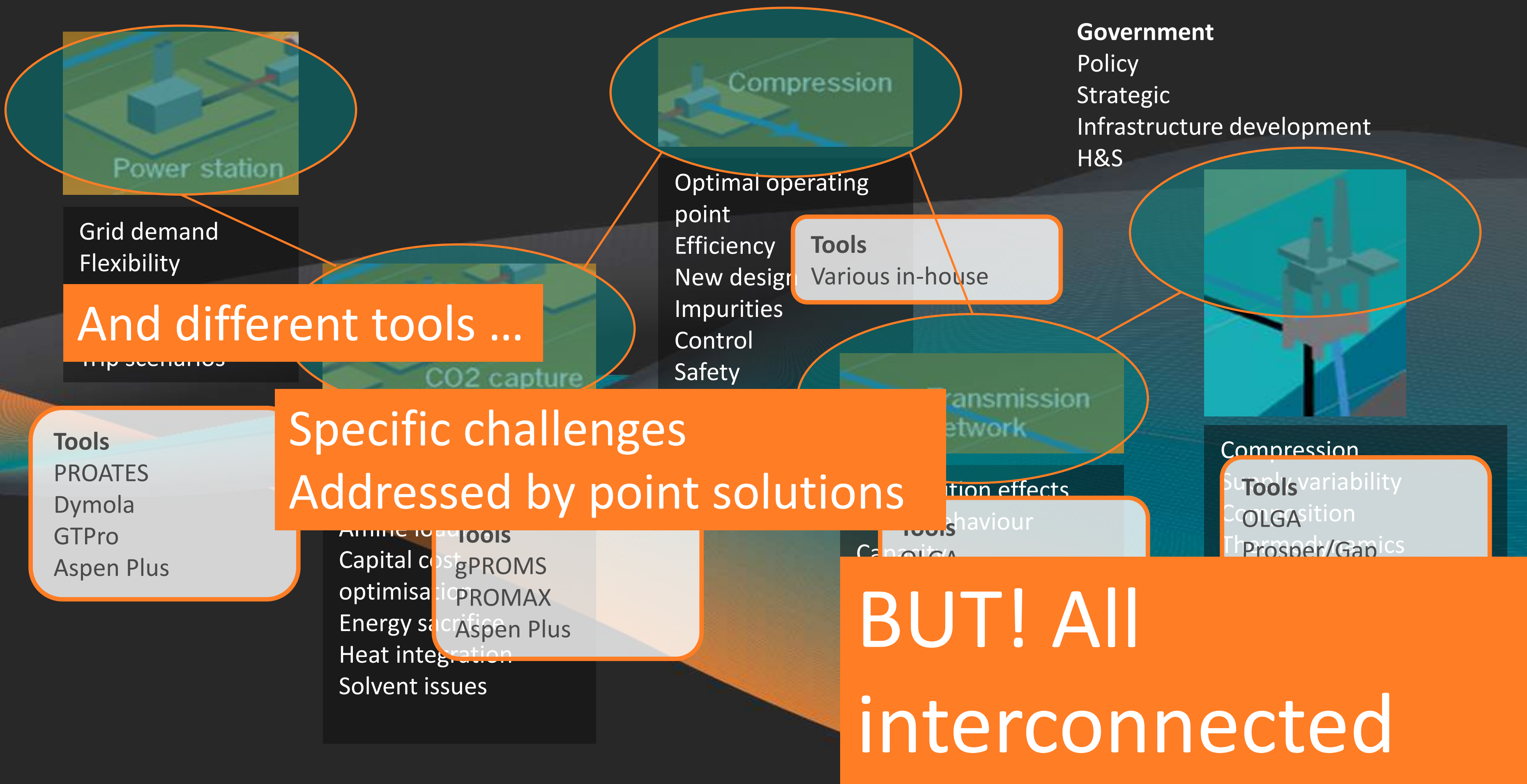
corporate

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

CCS challenges

# Each stakeholder has different issues & challenges



# An ETI-member survery revealed …

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

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

# Challenges – single site

## Post-combustion

Exit flow control?

CO2 breakthrough?

Energy integration - technicalities

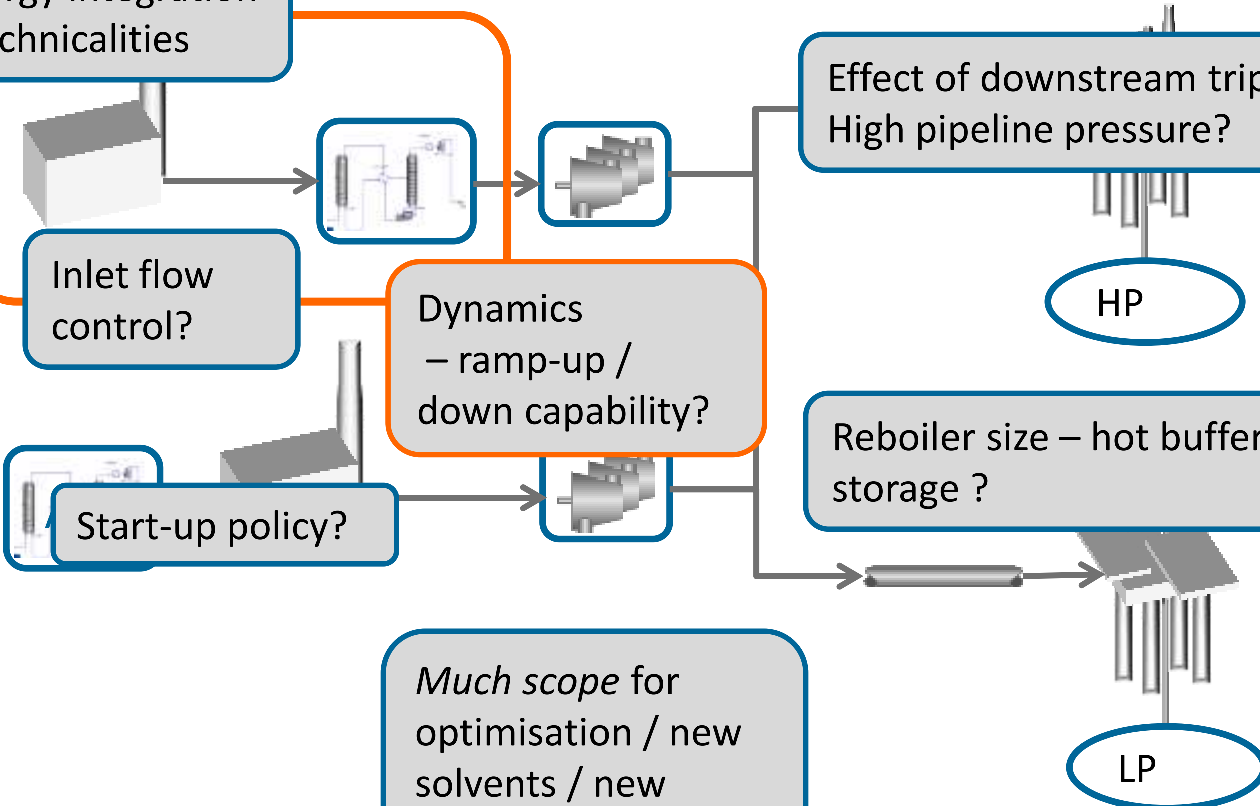
Effect of downstream trip?
High pipeline pressure?

Inlet flow control?

Dynamics – ramp-up / down capability?

Reboiler size – hot buffer storage ?

Start-up policy?




*Much scope* for optimisation / new solvents / new technologies

**Vent?**
How much? How long permitted? What is policy?

**Rich amine storage** – how much, when, where? Temperature?

**Energy integration** (energy penalty vs operability vs CAPEX)

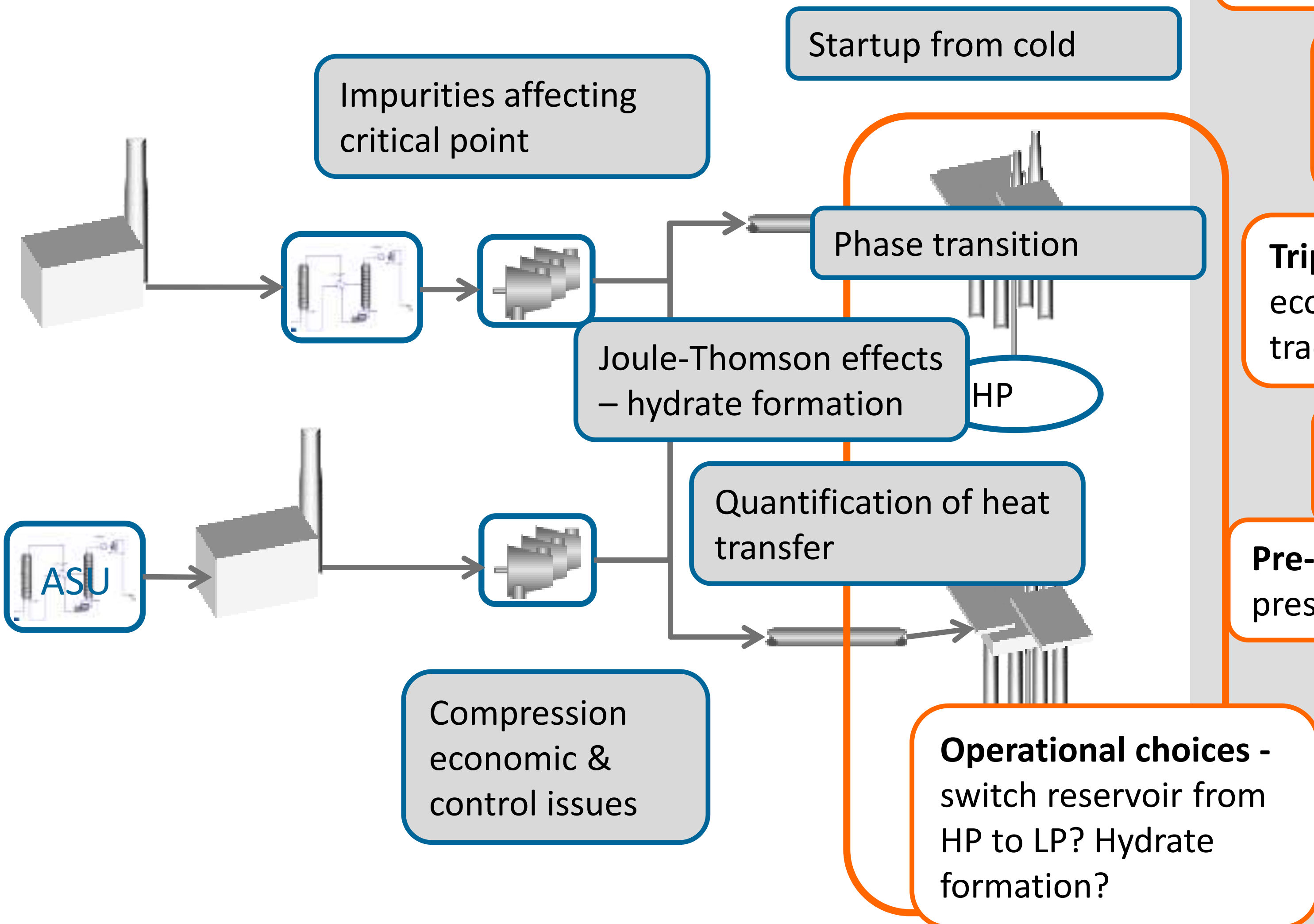
**Performance** of different capture technologies – amine vs caustic vs ?

By-pass economics

**Start-up** sequence – economic optimisation

# Many questions

## Injection & storage




**Phase considerations? Hydrate formation**

**HP v LP development economics**

**Trip scenarios** – economic effects and trade-offs

**Performance optimisation**

**Pre-injection heating** vs line pressurisation?

**Minimum & maximum rates**

**Safety**

# 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**

# CCS system modelling tool-kit project

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# System-wide modelling: Key enabling technology for CCS

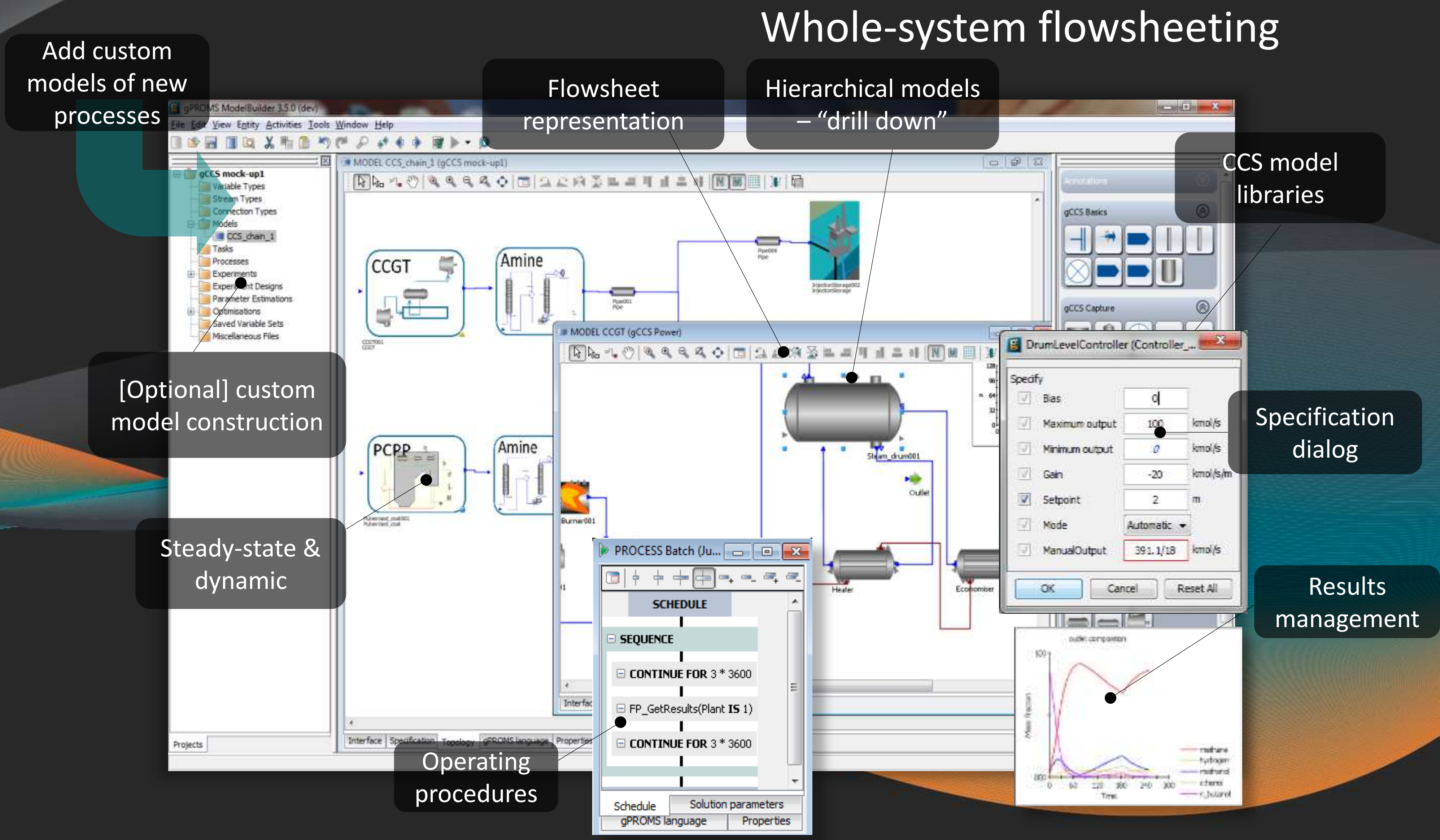
- **CCS System Modelling Tool-kit Project**
  - Energy Technologies Institute (ETI) £3m project
  - E.ON, EDF, Rolls-Royce, Petrofac/CO2DeepStore, PSE, E4tech

gPROMS modelling platform technology & expertise

Management

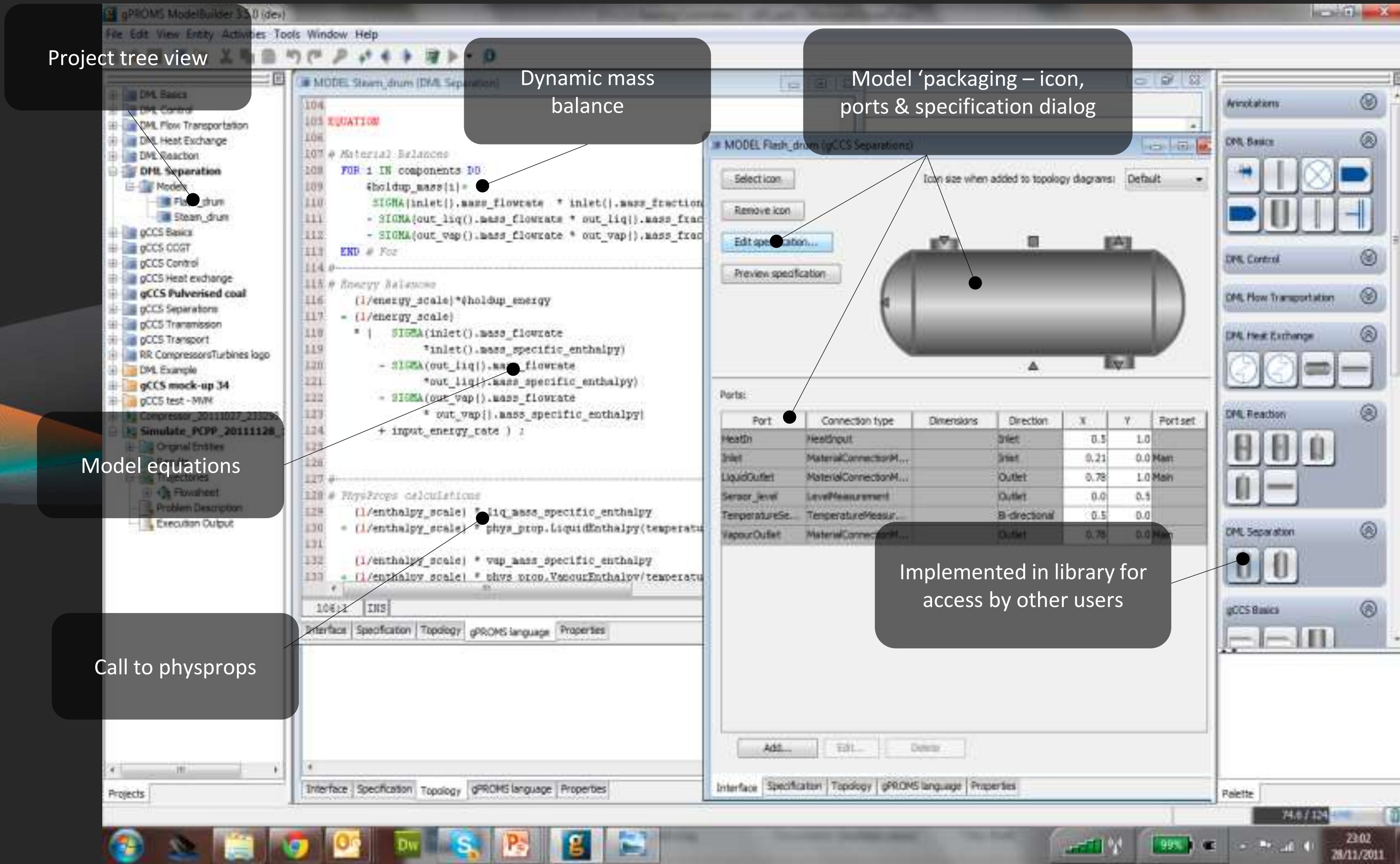
**→ Create a commercially available product**
- built on PSE's gPROMS platform
- High-fidelity system-wide CCS modelling
- Toolbox and ecosystem

# Environment – custom & system-wide modelling



# Environment – custom & system-wide modelling

## Powerful custom modelling

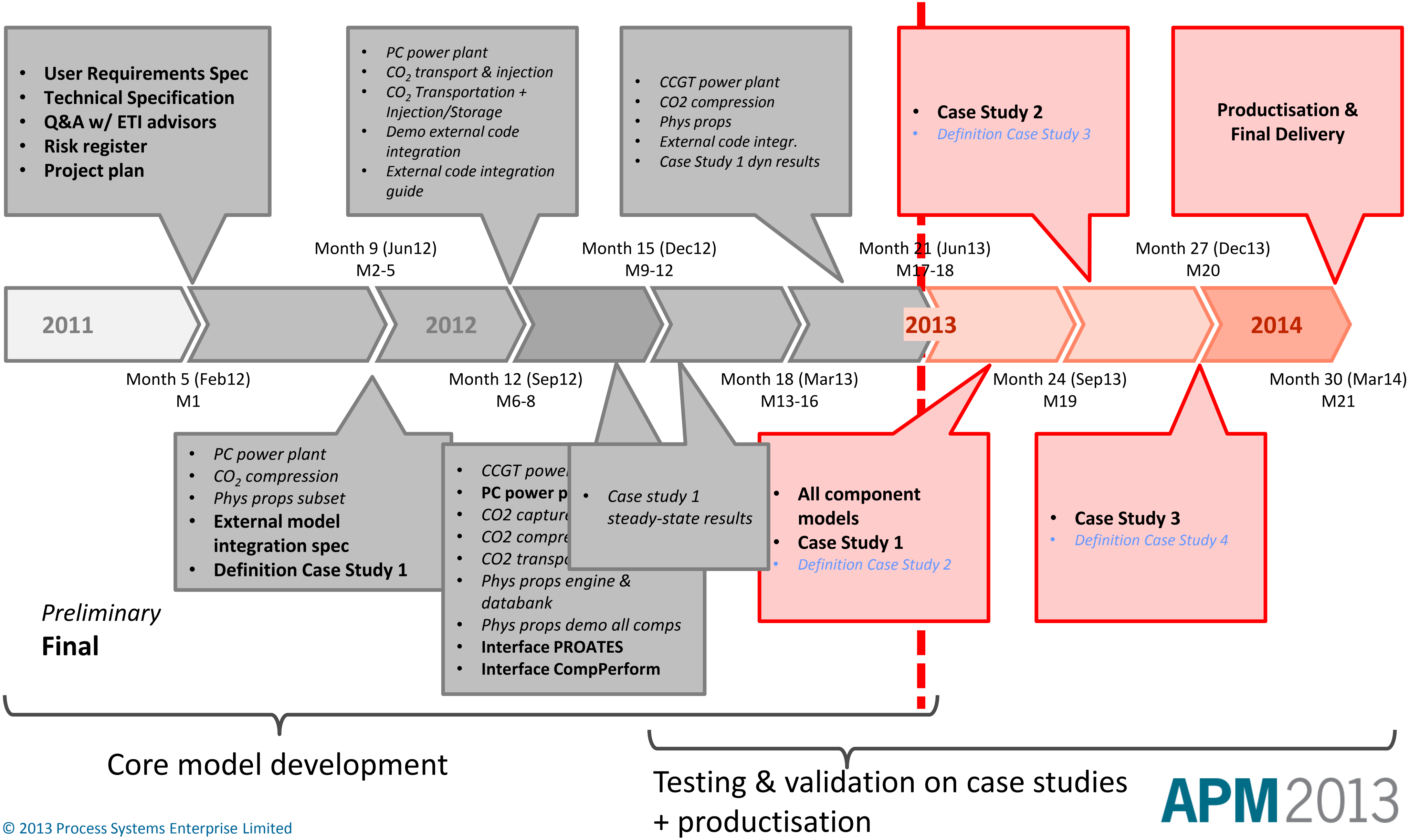


# Tool-kit components

## 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



User Requirements Spec
Technical Specification
Q&A w/ ETI advisors
Risk register
Project plan
PC power plant
$CO_2$ transport & injection
$CO_2$ Transportation + Injection/Storage
Demo external code integration
External code integration guide
CCGT power plant
CO2 compression
Phys props
External code integr.
Case Study 1 dyn results
Case Study 2
Definition Case Study 3
Productisation & Final Delivery
Month 9 (Jun12) M2-5
Month 15 (Dec12) M9-12
Month 21 (Jun13) M17-18
Month 27 (Dec13) M20
2011
2012
2013
2014
Month 5 (Feb12) M1
Month 12 (Sep12) M6-8
Month 18 (Mar13) M13-16
Month 24 (Sep13) M19
Month 30 (Mar14) M21
PC power plant
$CO_2$ compression
Phys props subset
External model integration spec
Definition Case Study 1
CCGT powe
PC power p
CO2 captur
CO2 compre
CO2 transp
Phys props engine & databank
Phys props demo all comps
Interface PROATES
Interface CompPerform
Case study 1 steady-state results
All component models
Case Study 1
Definition Case Study 2
Case Study 3
Definition Case Study 4
Preliminary
Final
Core model development
Testing & validation on case studies + productisation

# Tool-kit components / functionality

Model libraries

Physical properties

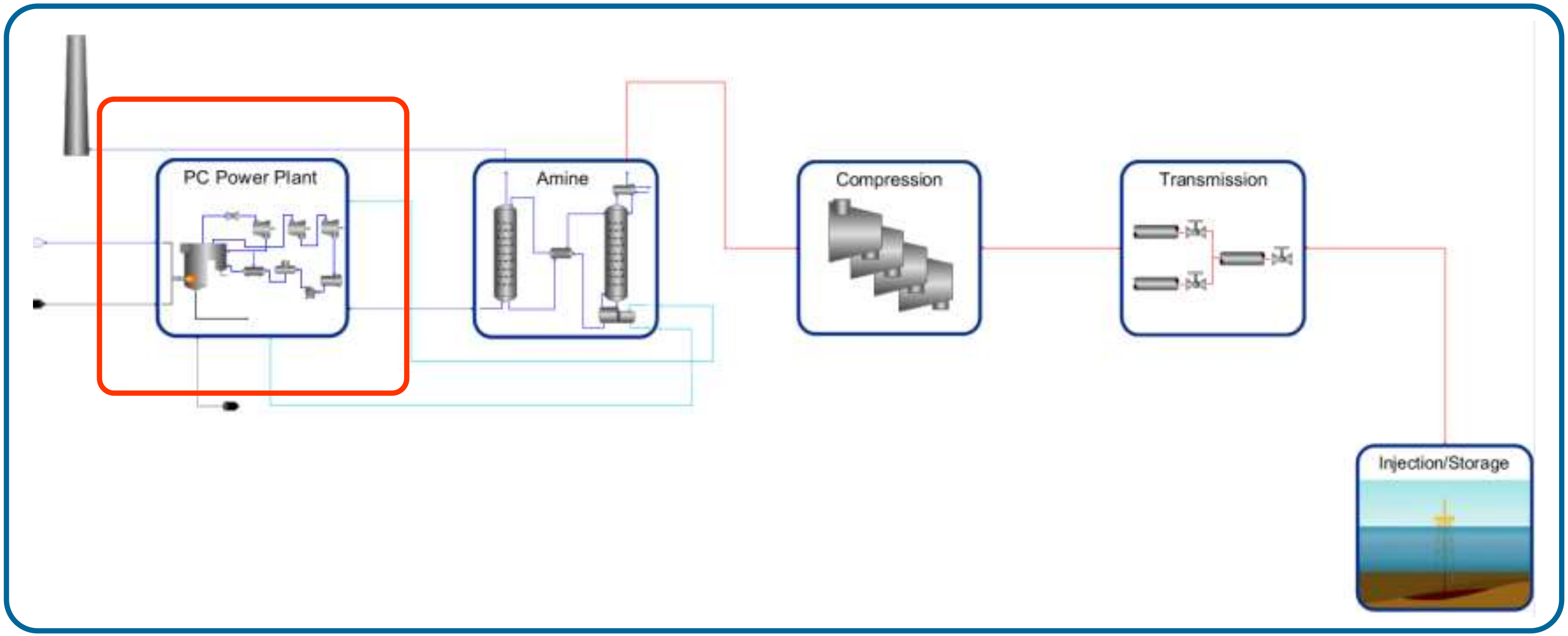
Interfaces

# 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.

# Power generation

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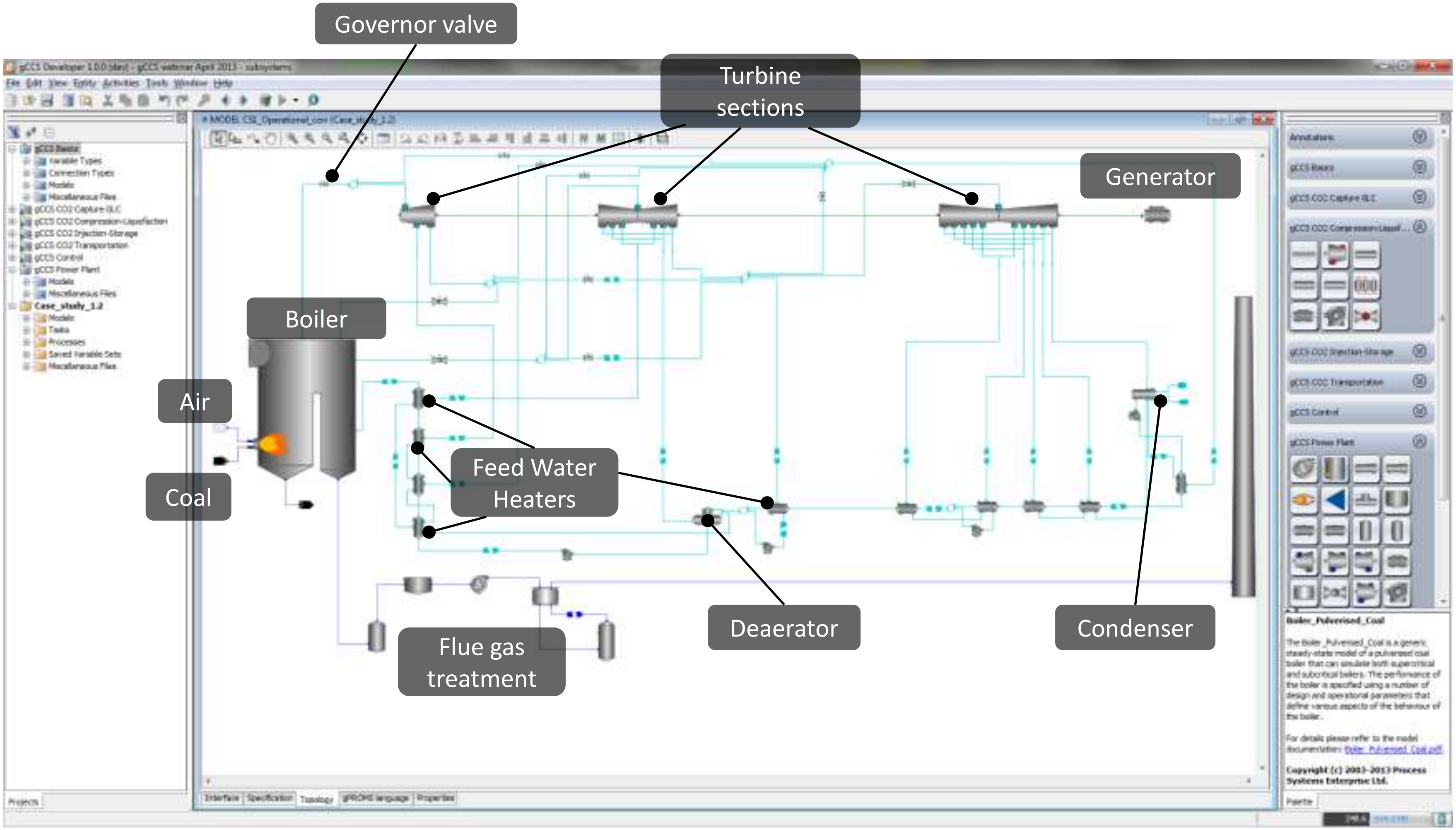
# Tool-kit components

## Model libraries – Power plant




Complex flowsheet with > 10 recycles & a closed loop:

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

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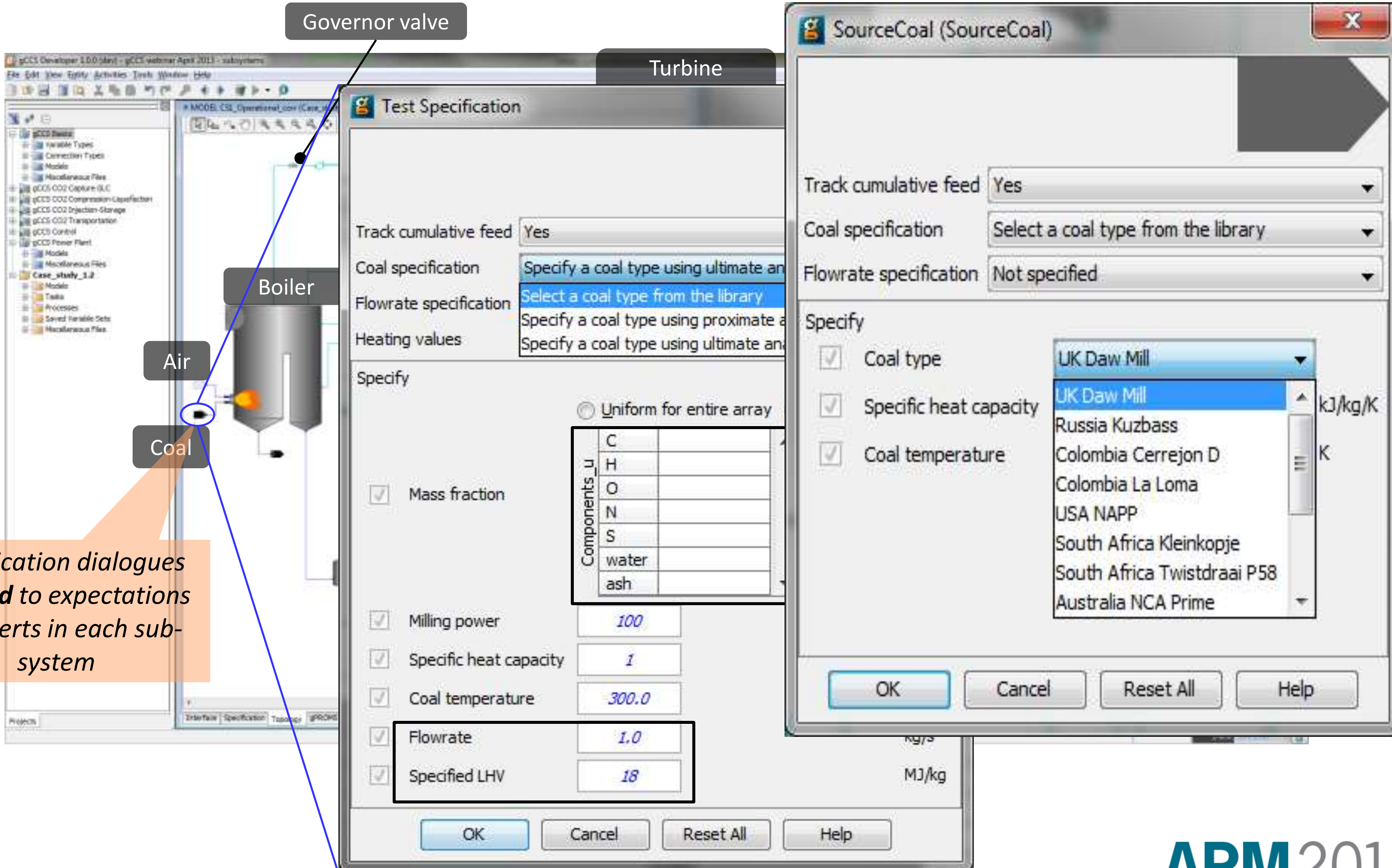
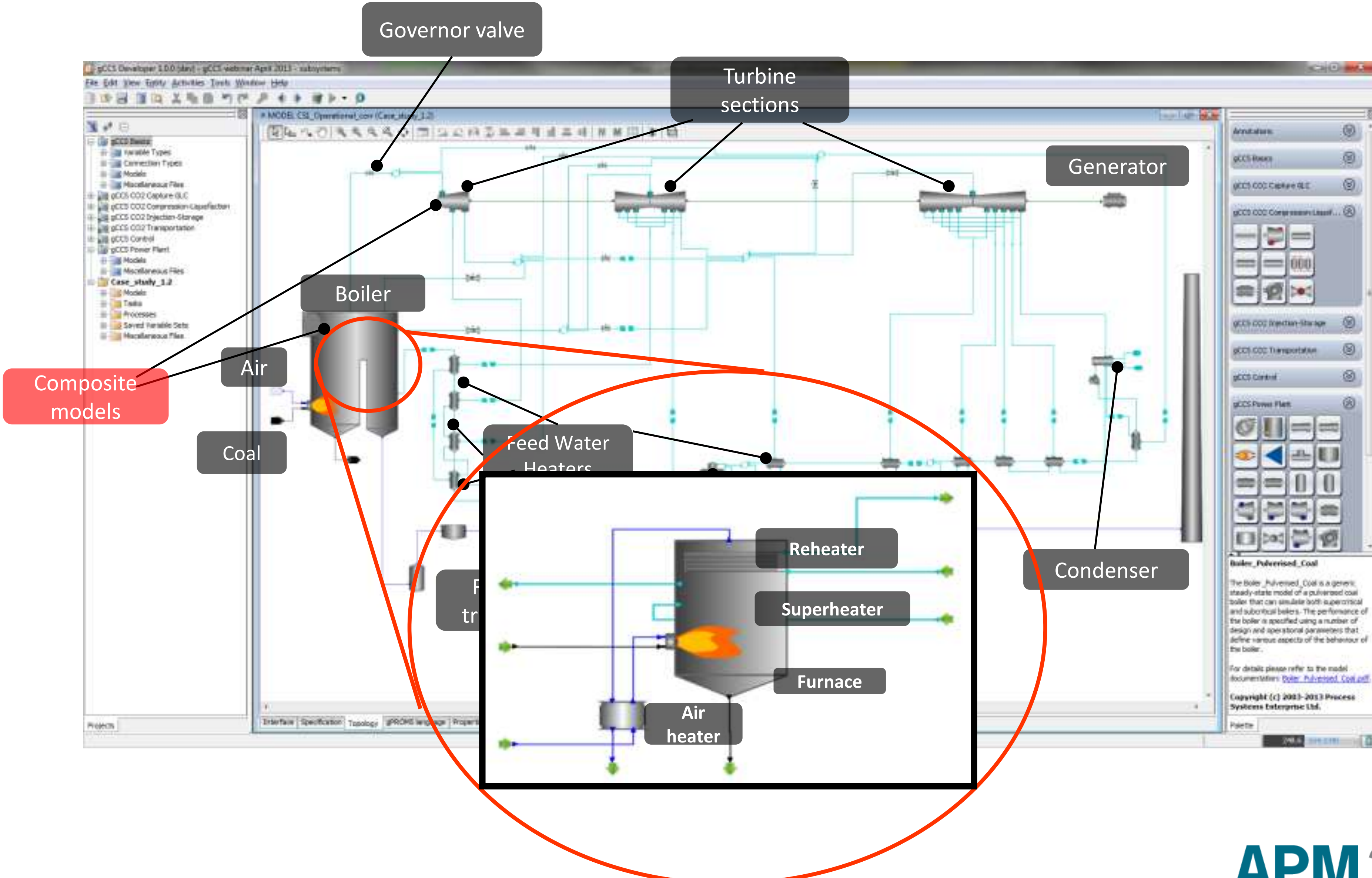
# Tool-kit components

## Model libraries – Power plant




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

# PCPP library overview: Whole PCPP

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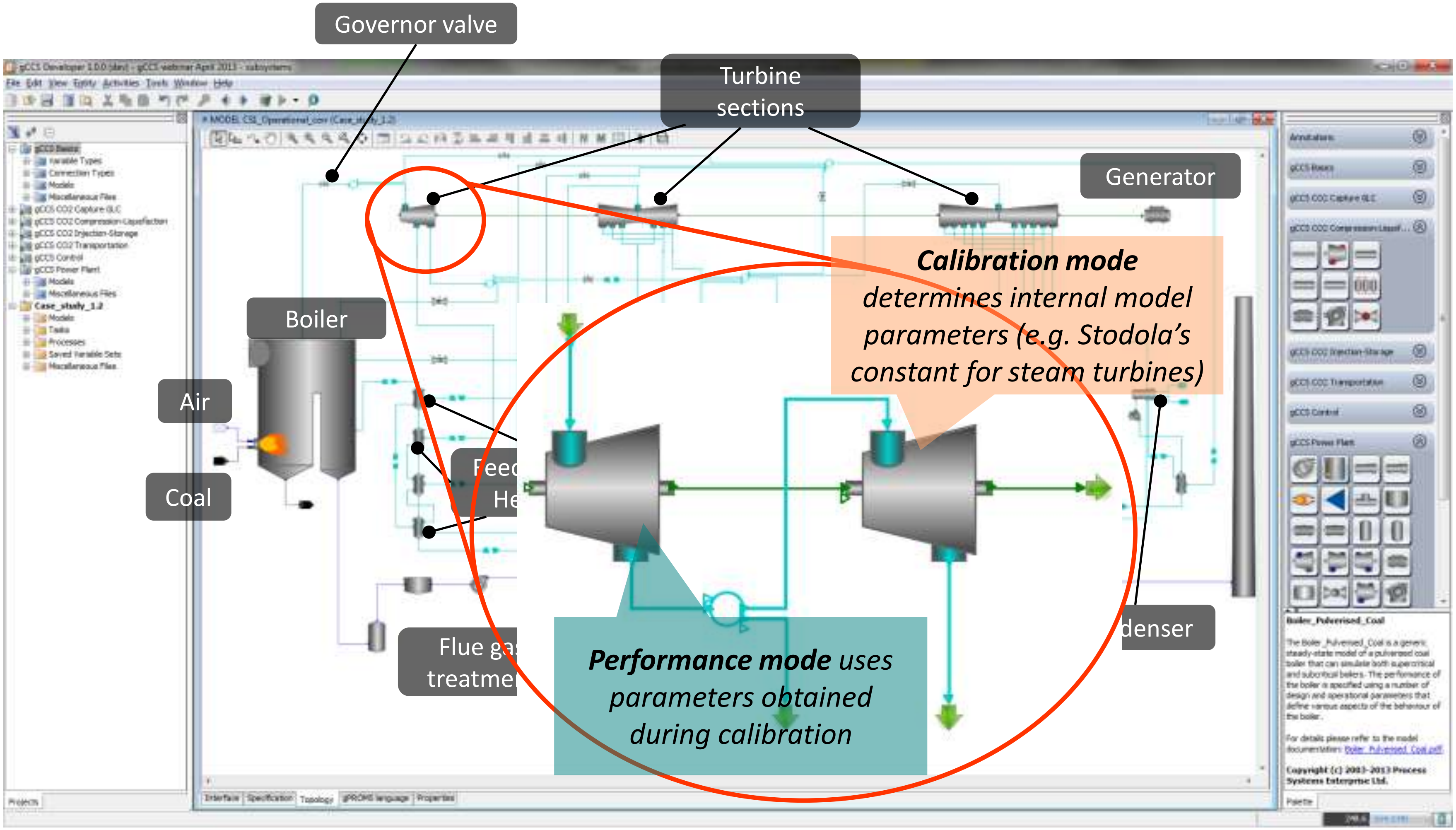
# Tool-kit components

## Model libraries – Power plant

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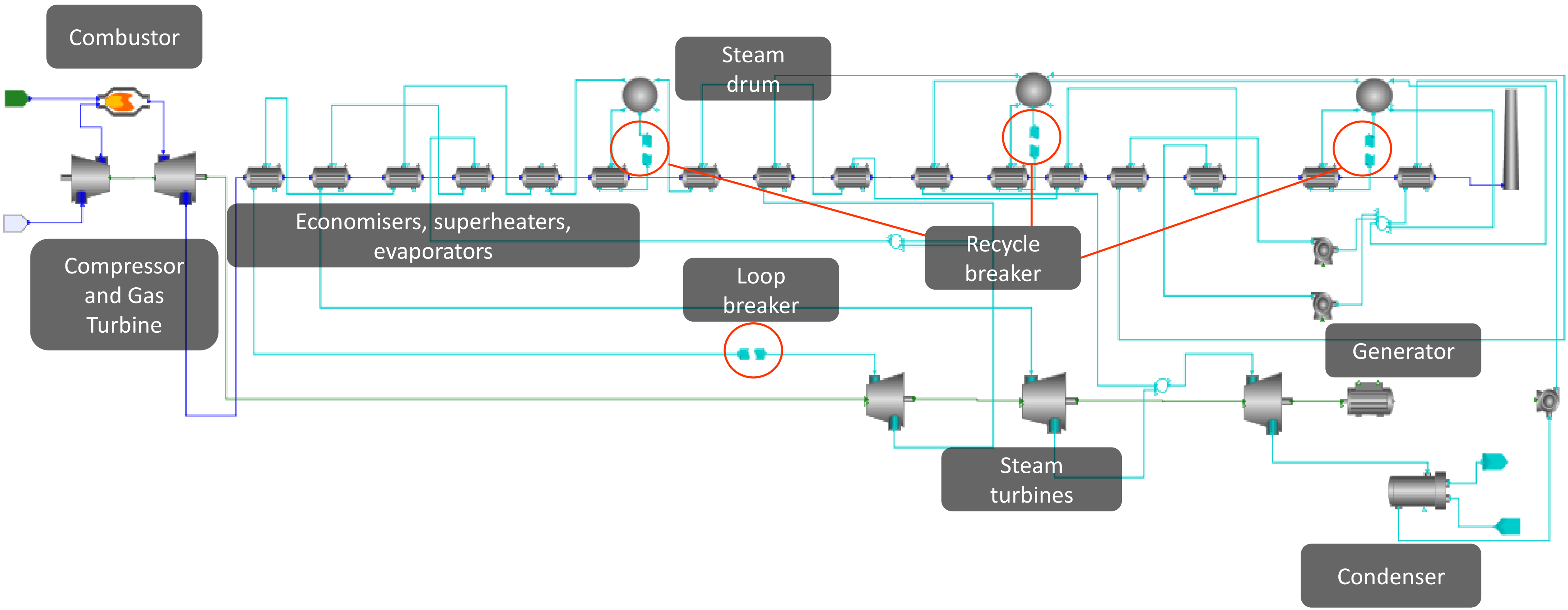
- Combined Cycle Gas Turbine flowsheet

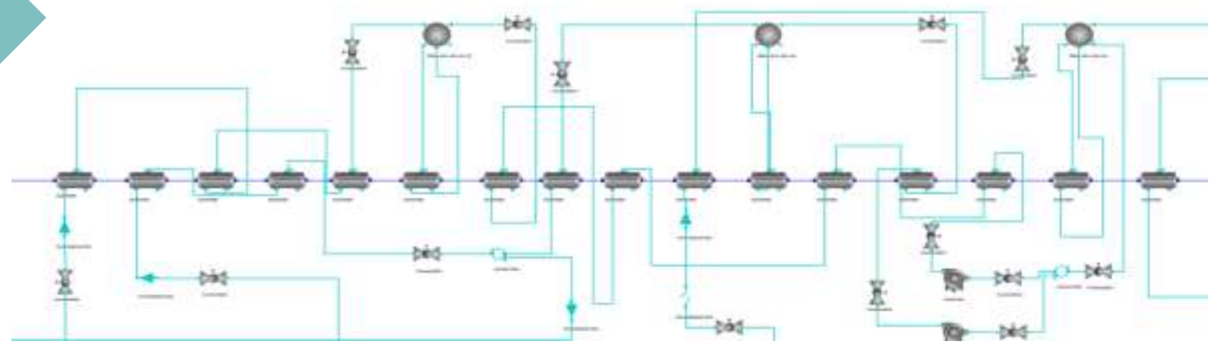


# Tool-kit components

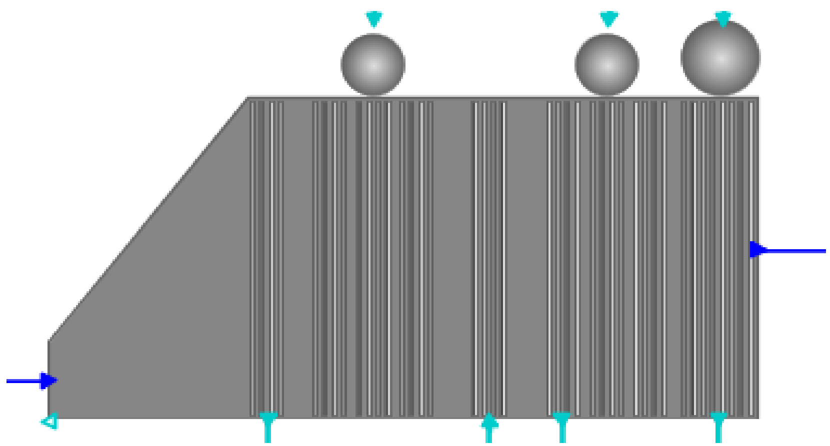
## Model libraries – Power plant

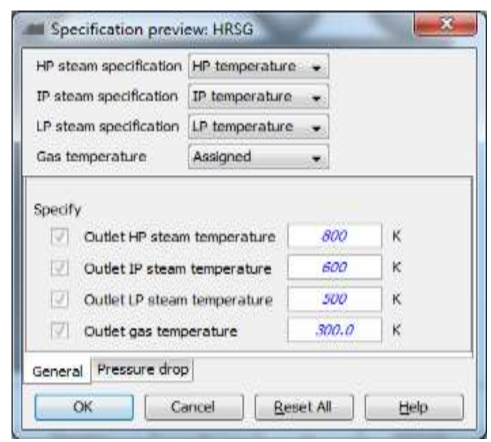
- High fidelity model of HRSG
  - comprising multiple units
  - predictive at part-load
- High level (low fidelity) model
  - Single unit model
  - Not predictive at part-load (temperatures are inputs)

Detailed HRSG model



High level model



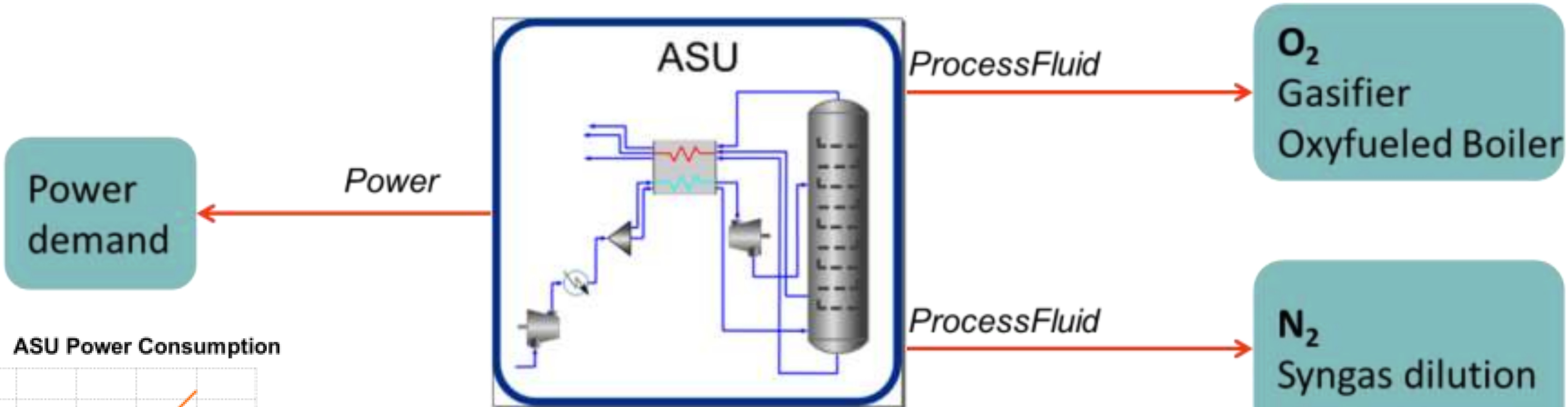


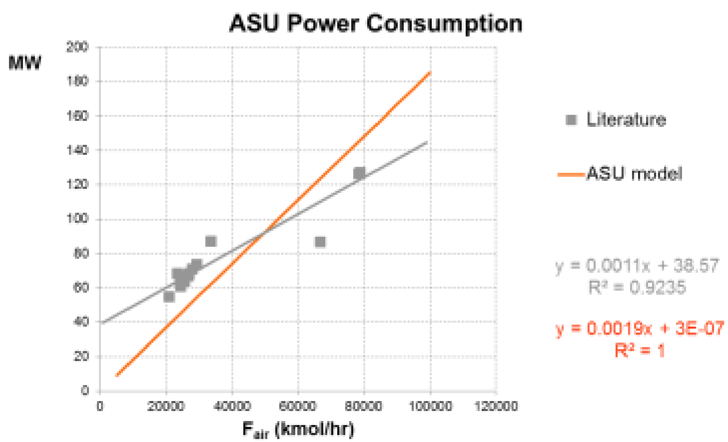
# Tool-kit components

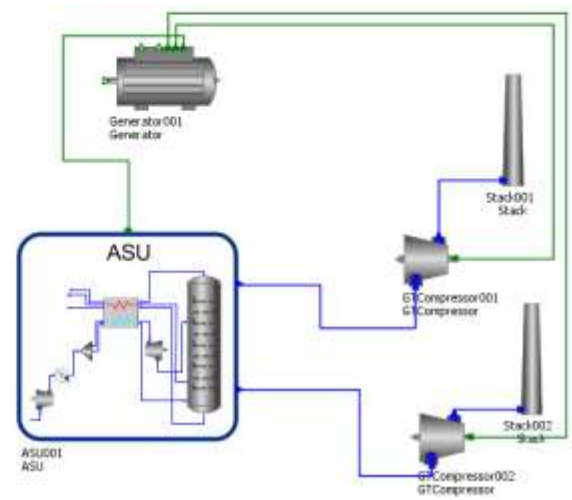
## Model libraries – Power plant

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

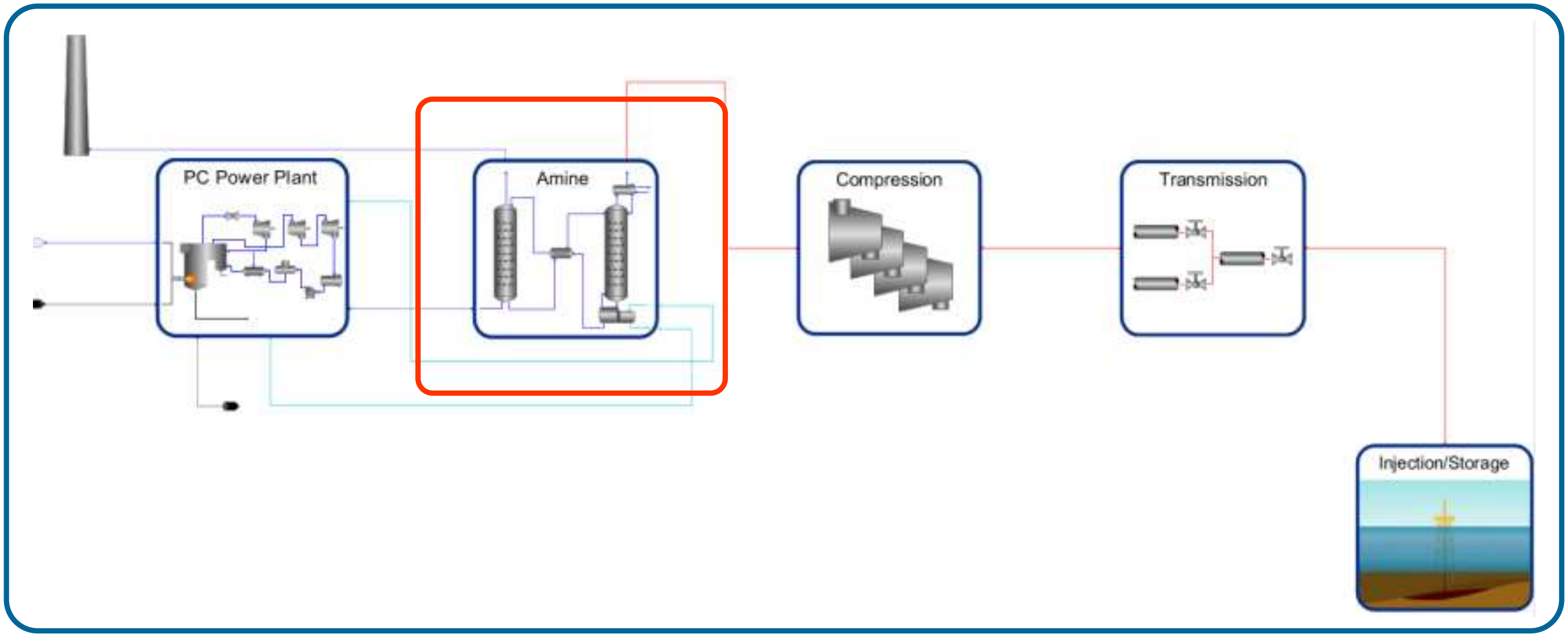
**Model acts as Source of $O_2$ and $N_2$ and calculates power demand**



# Power generation

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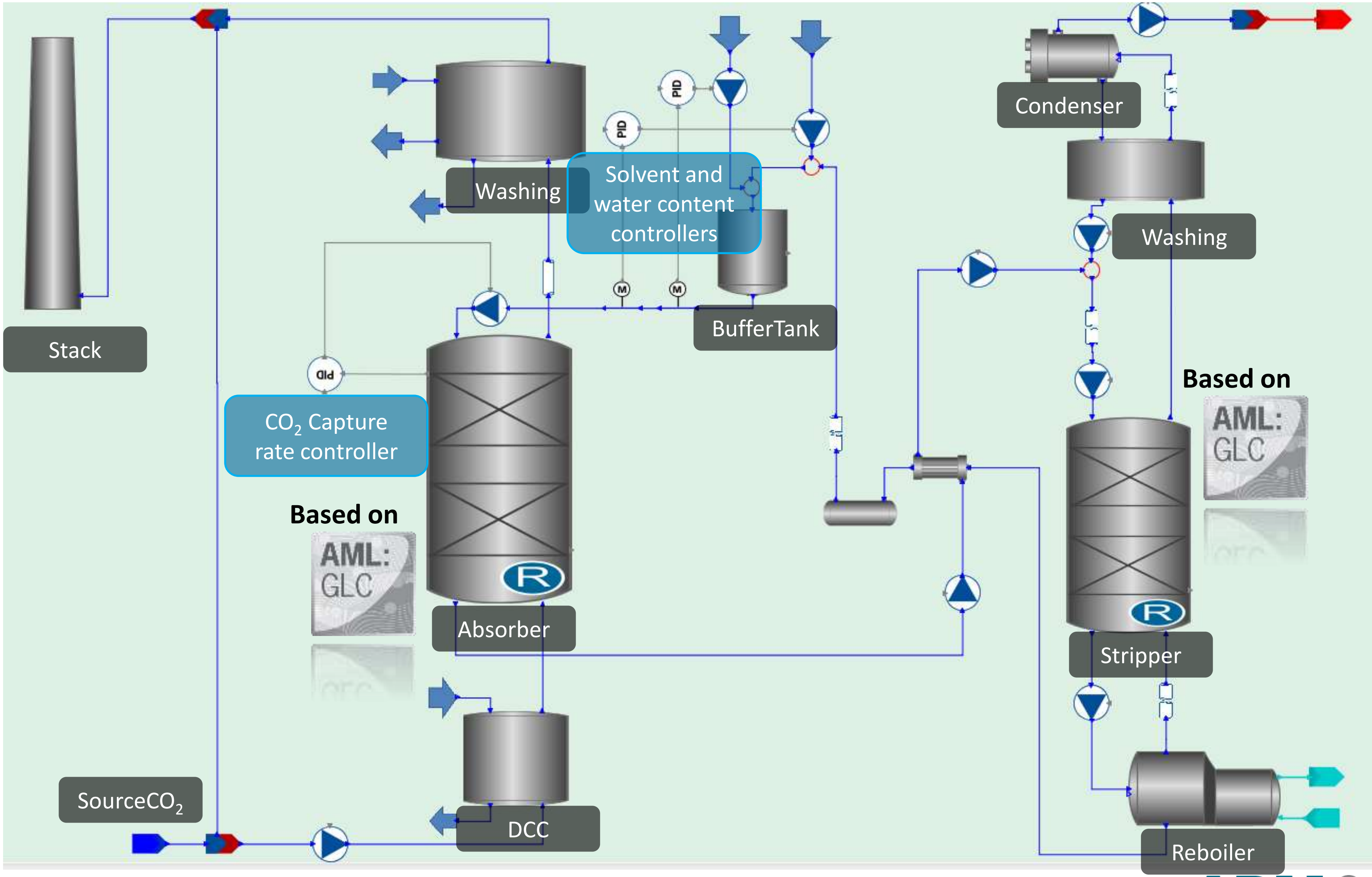
# Tool-kit components

## Model libraries – $CO_2$ Capture (chemical and physical absorption)

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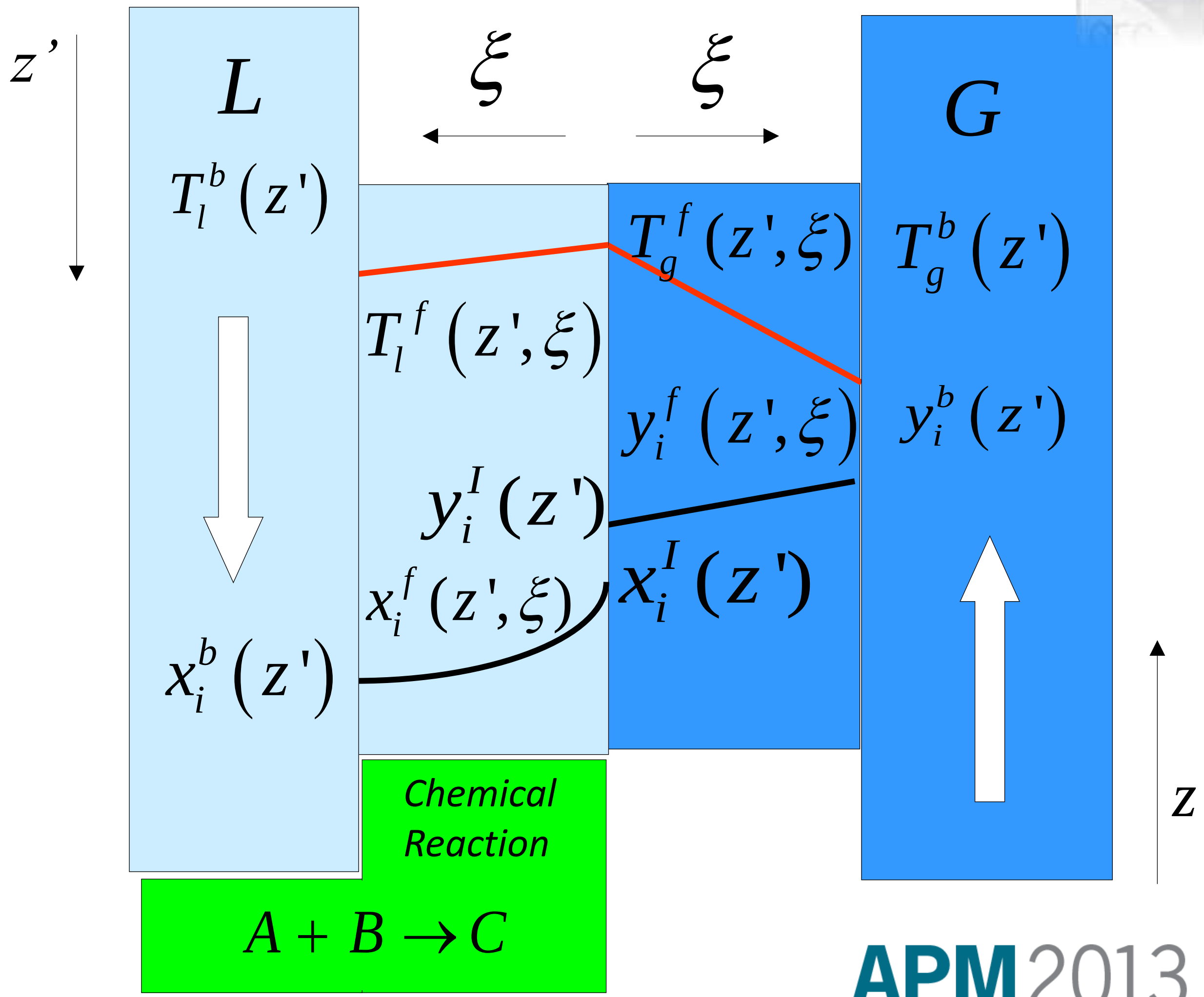
- Non-equilibrium models
- Models distributed in axial direction and in the direction of the liquid and vapour films
- Energy balance and V/L equilibrium at the interface
- Phase behaviour and chemical equilibrium <u>currently</u> calculated by OLI thermodynamic package
  - to be replaced by gSAFT
-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



# Tool-kit components

## Model libraries – $CO_2$ Capture: *Modelling of ionic reactions in gas/liquid separation*

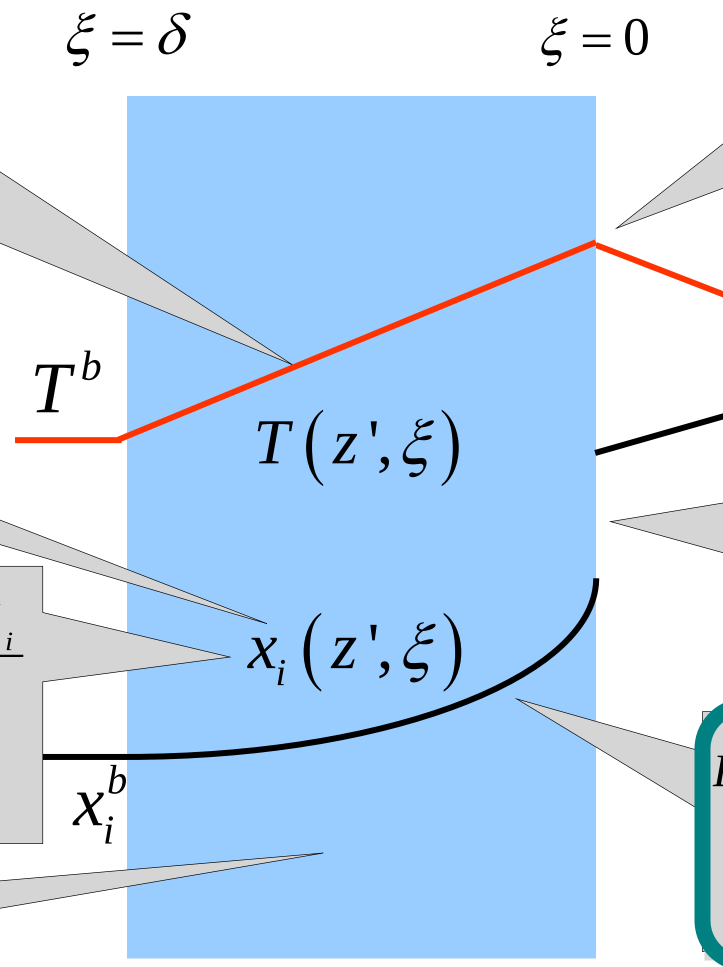
$$\frac{\partial}{\partial z'}\left(\lambda \frac{\partial T}{\partial z'}\right) + \boxed{\sum_{j=1}^{n_l}\left(-\Delta H^{R}{}_{j} R_j\right)} = \frac{\partial}{\partial z'}\left(\sum_{i=1}^{n_l} N_i H_i\right)$$

$$\frac{\partial N_i}{\partial z'} = \boxed{G_i} \quad i = 1,\dots,n_l$$

$$-\frac{x_i}{RT}\frac{\partial \mu_i}{\partial \xi} \boxed{- x_i z_i \frac{F}{RT}\frac{\partial \Phi}{\partial \xi}} = \sum_{\substack{k=1 \\ k\neq i}}^{n_l} \frac{x_i N_k - x_k N_i}{c_t D_{ik}}$$

$$i = 1,\dots,(n_l - 1)$$

$$\sum_{i=1}^{n_l} x_i = 1 \qquad \boxed{\sum_{i=1}^{n_l} x_i z_i = 0}$$




$$T_l^I = T_g^I$$

$$-q_g^I = q_l^I + \sum_{i=1}^{n_{VLE}} N_i^I \lambda_i$$

$$K_i^{VLE} = \frac{f_i^I\big|_g}{f_i^I\big|_l}$$

$$N_i^I\big|_l = -N_i^I\big|_g$$

$$i = 1,\dots,n_{VLE}$$

$$\boxed{\begin{aligned} R_i &= k_i \prod_j C_j^l \quad i = 1,\dots,n_R \\ G_i &= \sum_j \nu_{ij} R_j \end{aligned}}$$

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# Tool-kit components

## Model libraries – $CO_2$ Capture

$H_2O$ ⬄ H(+) + OH(-)

$HCO_3$(-) + OH(-) ⬄ $CO_3$(-) + H2O

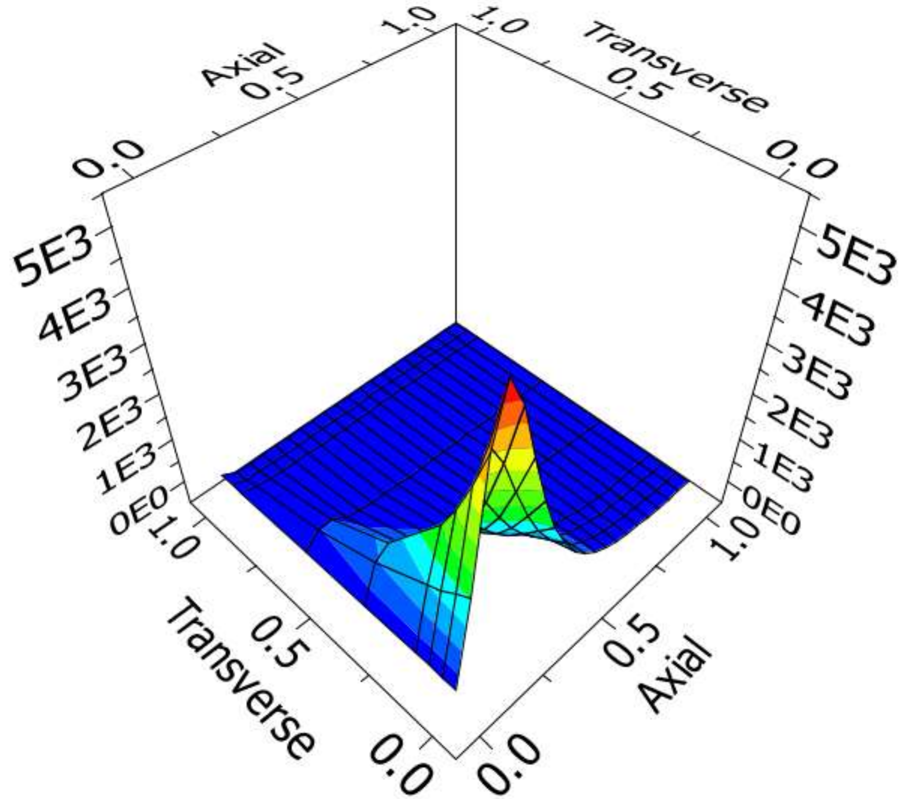
$CO_2$ + OH(-) ⬄ $HCO_3$(-)

**$CO_2$ + MEXH ⬄ $MEXCO_2$(-) + H(+)**

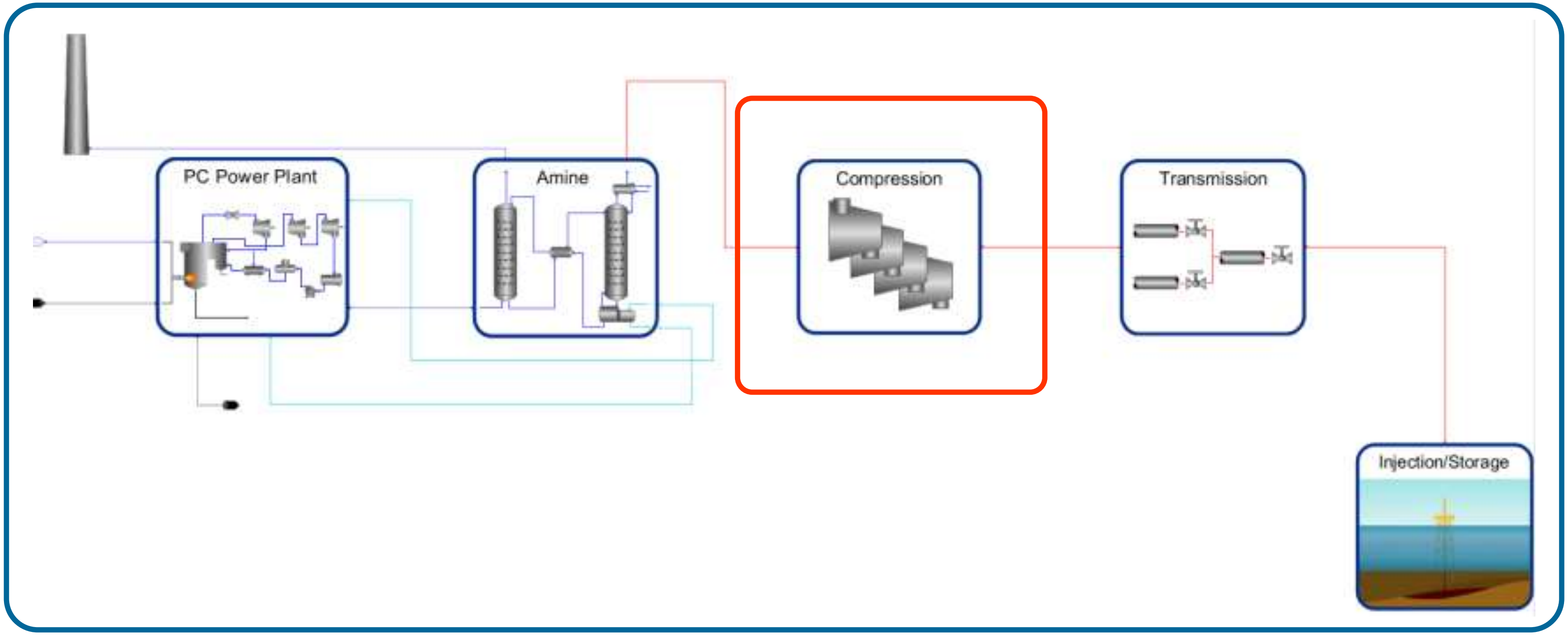
MEXH + H2O ⬄ $MEXH_2$(+) + OH(-)

Carbamate formation,
kinetically controlled reaction

Transversal and axial profiles for the reaction rate of carbamate formation



# Compression

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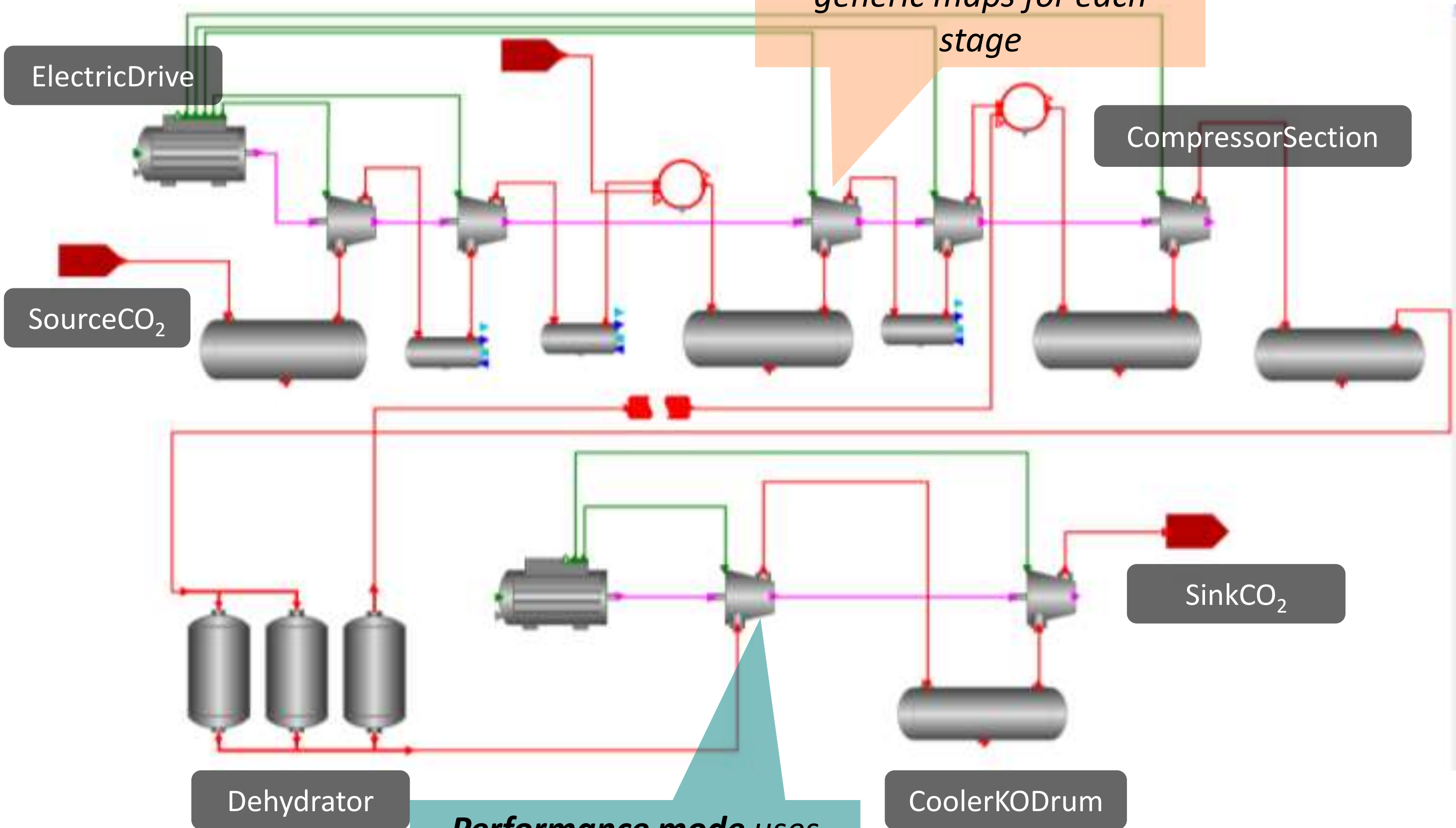
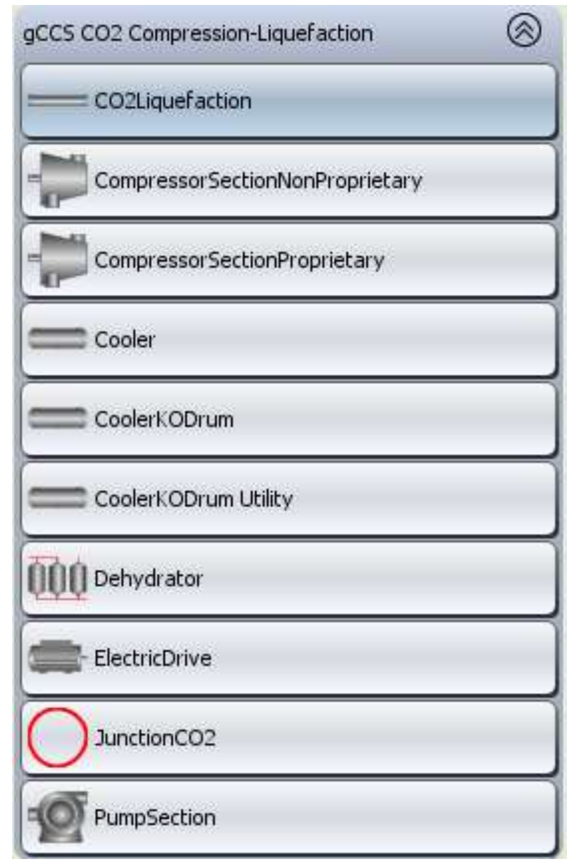
# Tool-kit components

## 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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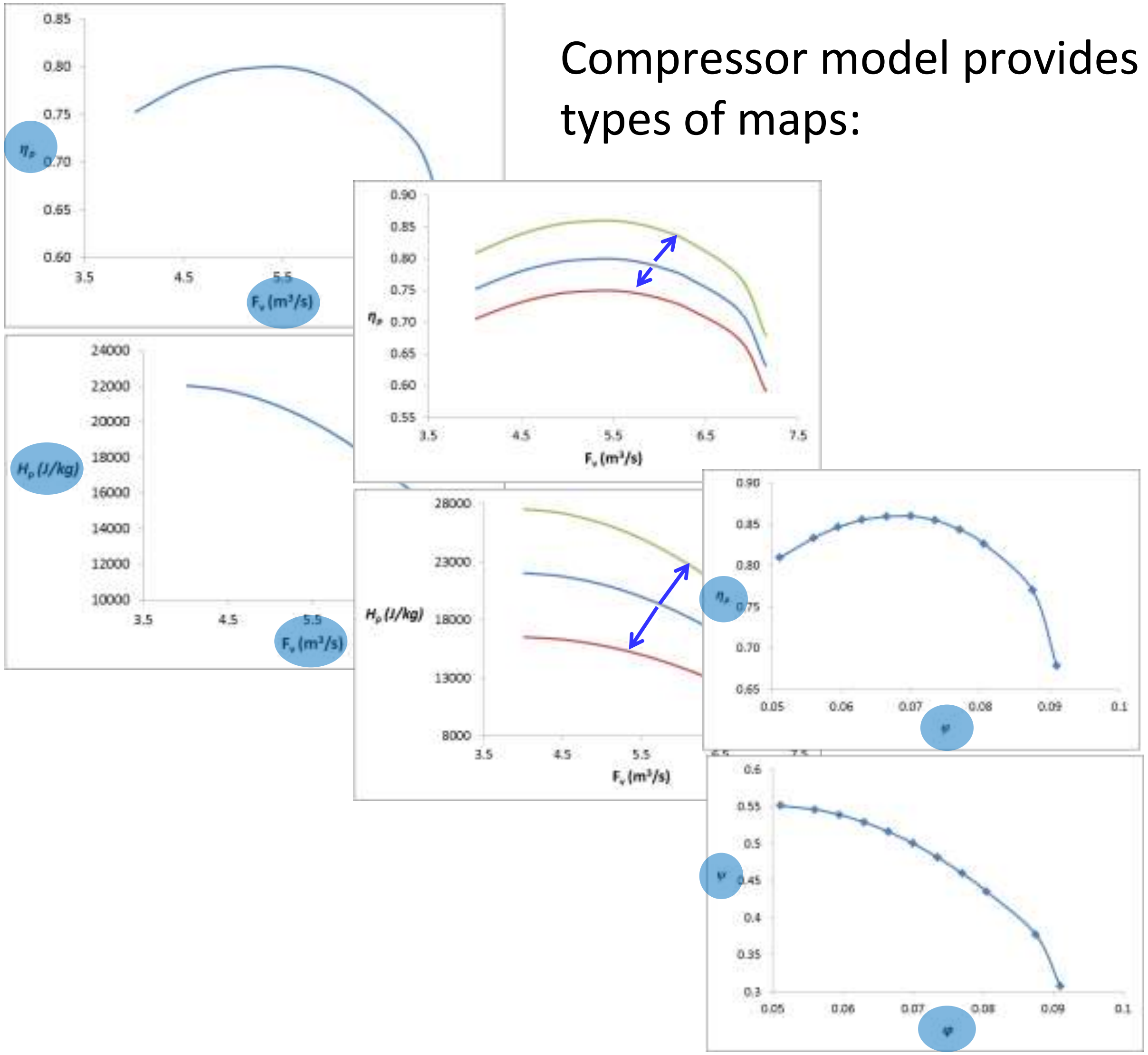
# Tool-kit components

## Model libraries – $CO_2$ Compression & Liquefaction




$\varphi = 4F_v / (D^2 v)$

$\psi = H_p / v^2$

Compressor model provides the specification of three different types of maps:

- **1D maps**
  - Efficiency/flow curve
  - Head/Flow curve
  - Uses affinity laws to extrapolate for different speeds
- **2D maps**
  - Same curves as 1D maps
  - One curve for each speed
  - Interpolates between the curves to determine operation for different speeds
- **Dimensionless maps**
  - Curve based on dimensionless flow (φ) and head (ψ)
  - Contains same information as 2D maps

## Operational studies – control: Surge avoidance

- Increase volumetric flowrate in the compressor
  - Recycle compressed flow to the inlet through a recycle loop

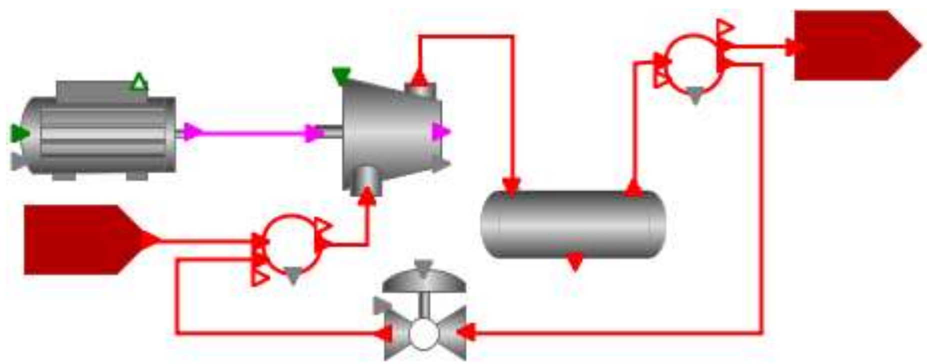


Fig. 4 – Cooled recycle loop used in surge control.

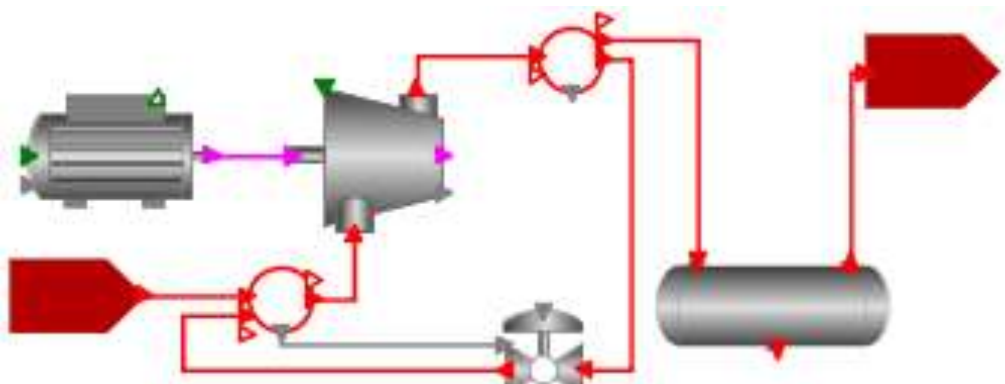
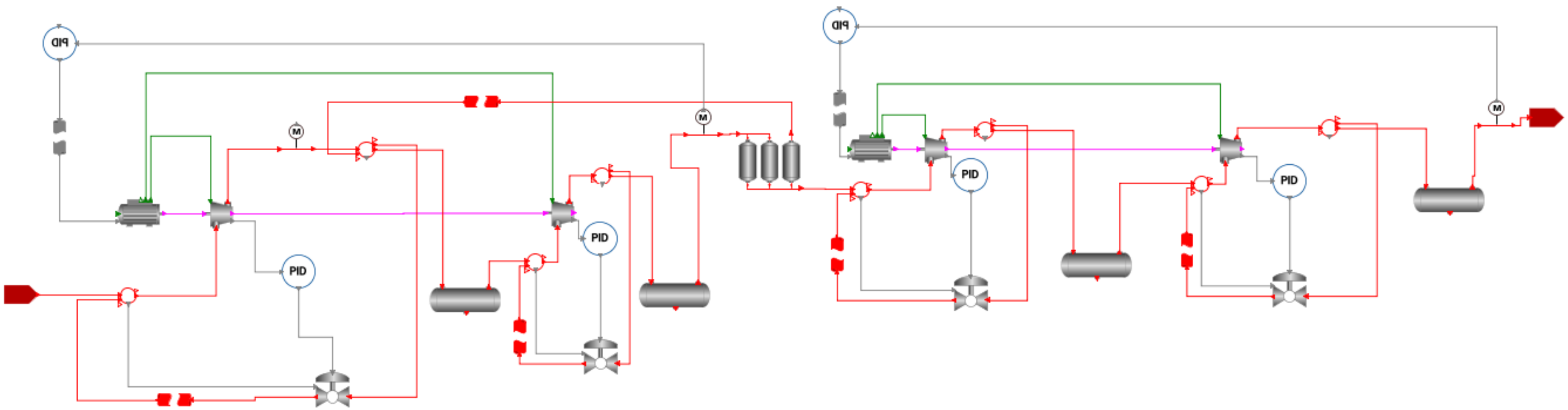
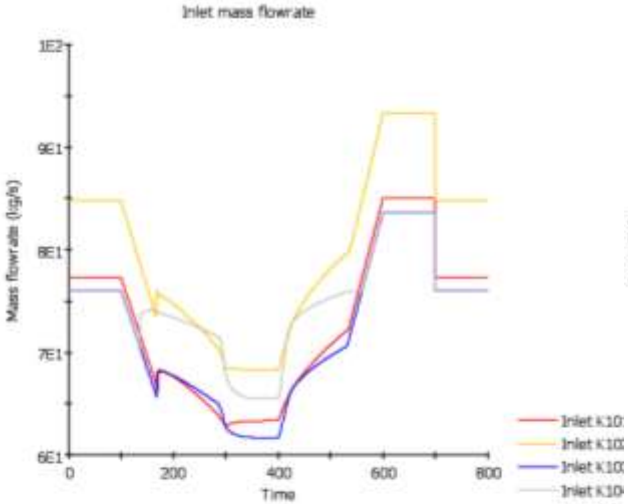


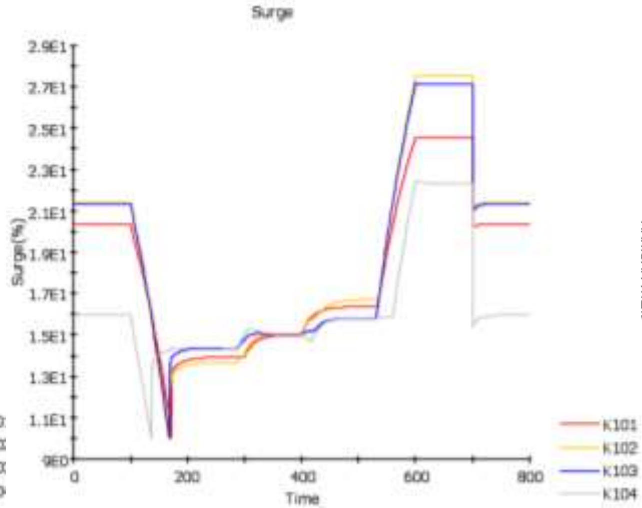
Fig. 5 – Non-cooled recycle loop used in surge control.

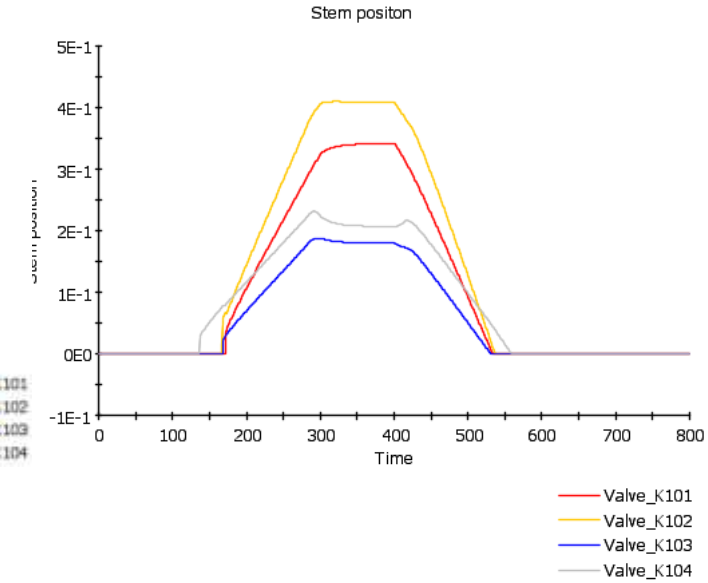
# Tool-kit components

## Model libraries – $CO_2$ Compression & Liquefaction



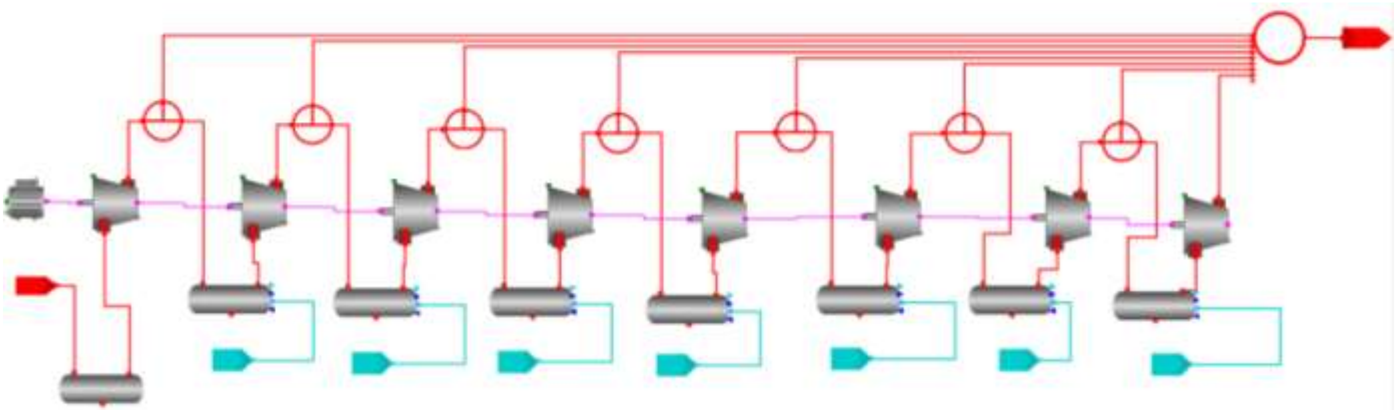



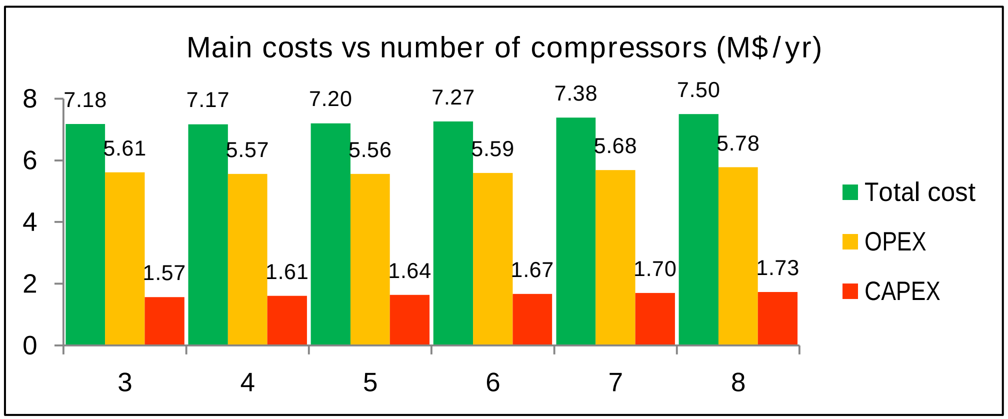



# Tool-kit components – Advanced features

## Model libraries – $CO_2$ Compression & Liquefaction

### Compression train - design optimisation






1. Detailed $CO_2$ Compression library models
   \+
   gPROMS mixed integer/continuous optimisation
   ➔ **full compression train design optimisation**
2. Techno-economical design to minimise total cost
   **CAPEX + OPEX**
3. Determine
   1. number of compressors & coolers
   2. design parameters (impeller diameters; HT areas)

   that are optimal for **a set of operating scenarios** (different $CO_2$ flows and final discharge pressures)

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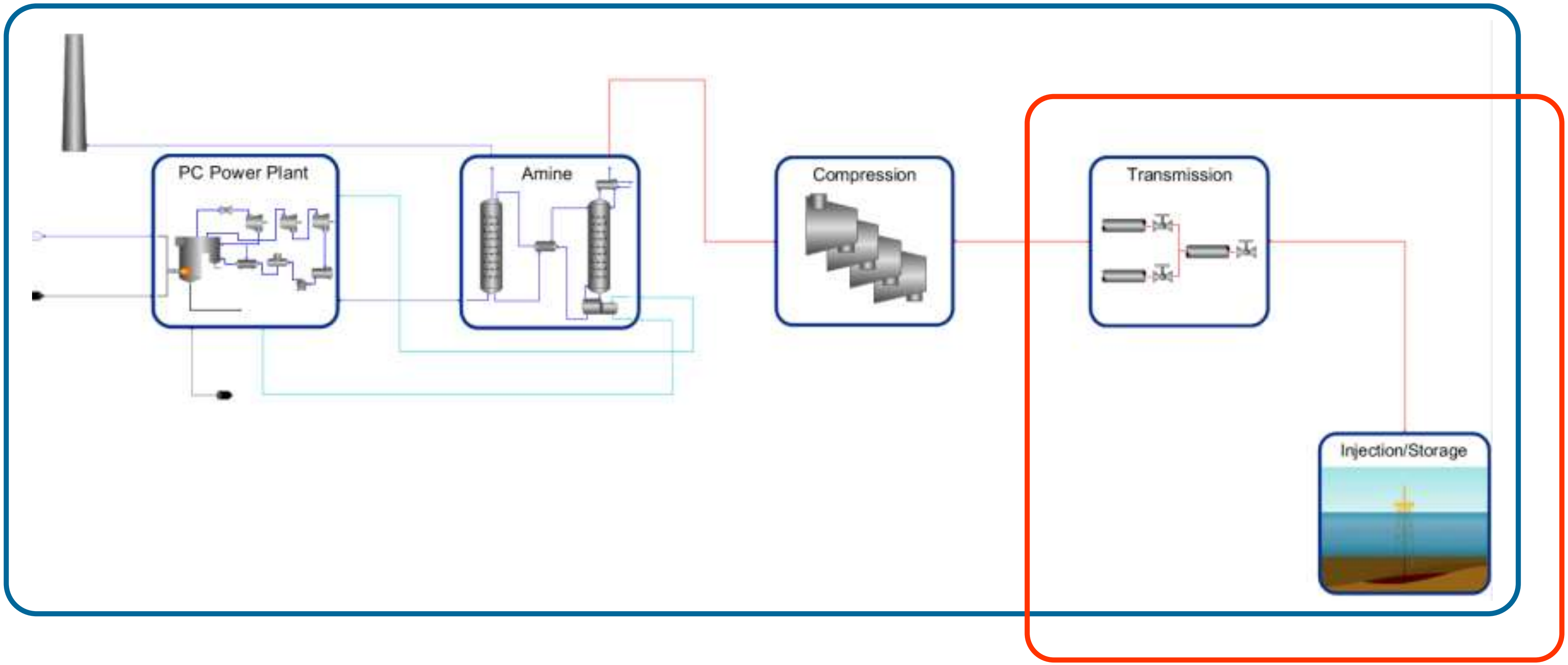
# Transmission & injection

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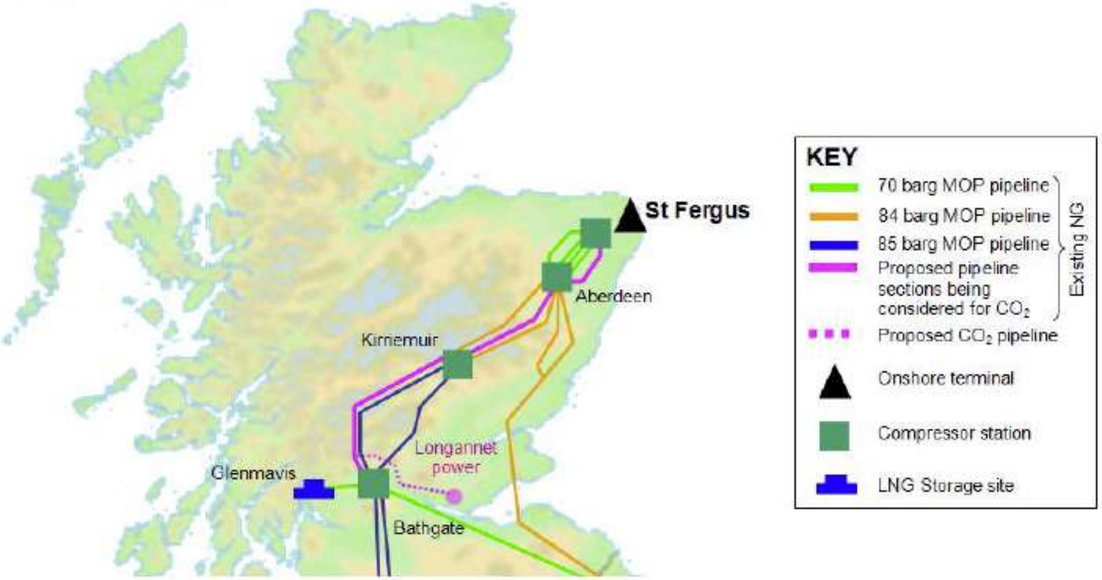
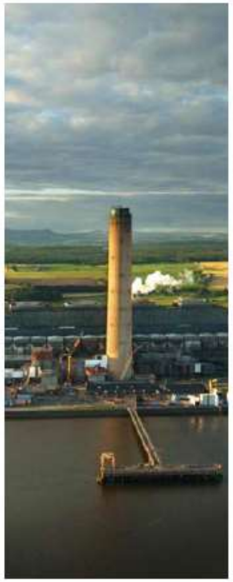
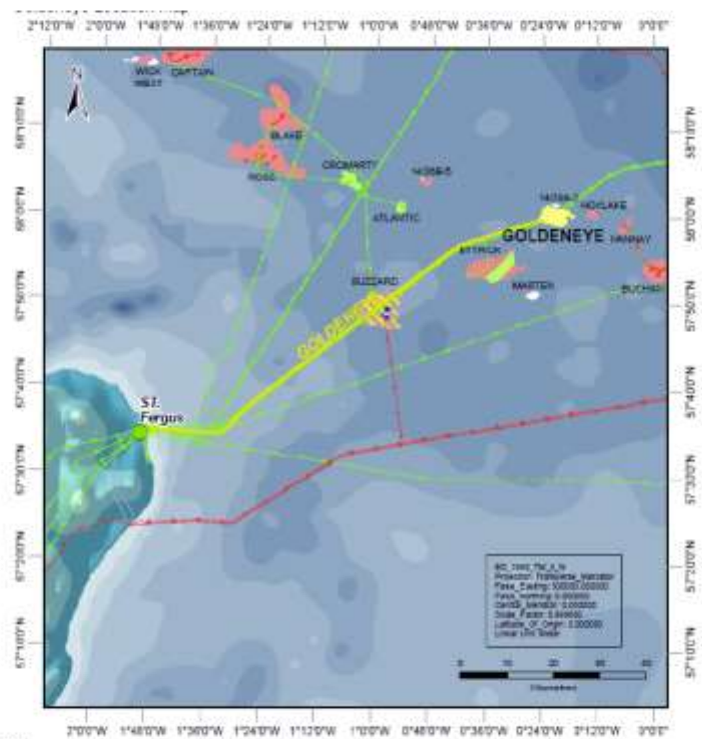
# Transmission and injection sub-system
## Components of the CCS chain




Source: National Grid






Source: Shell



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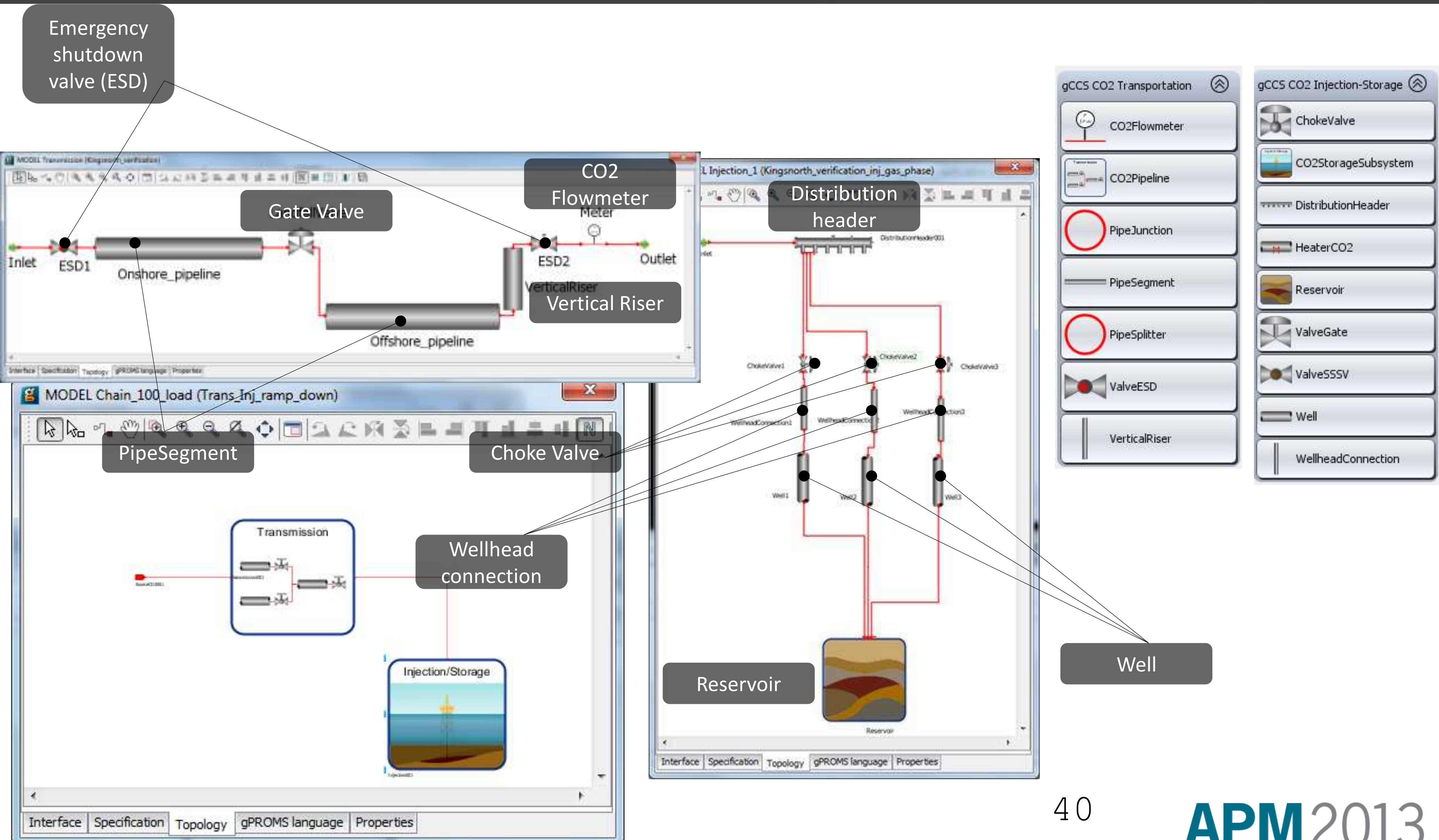
# Transmission and Injection – Component models



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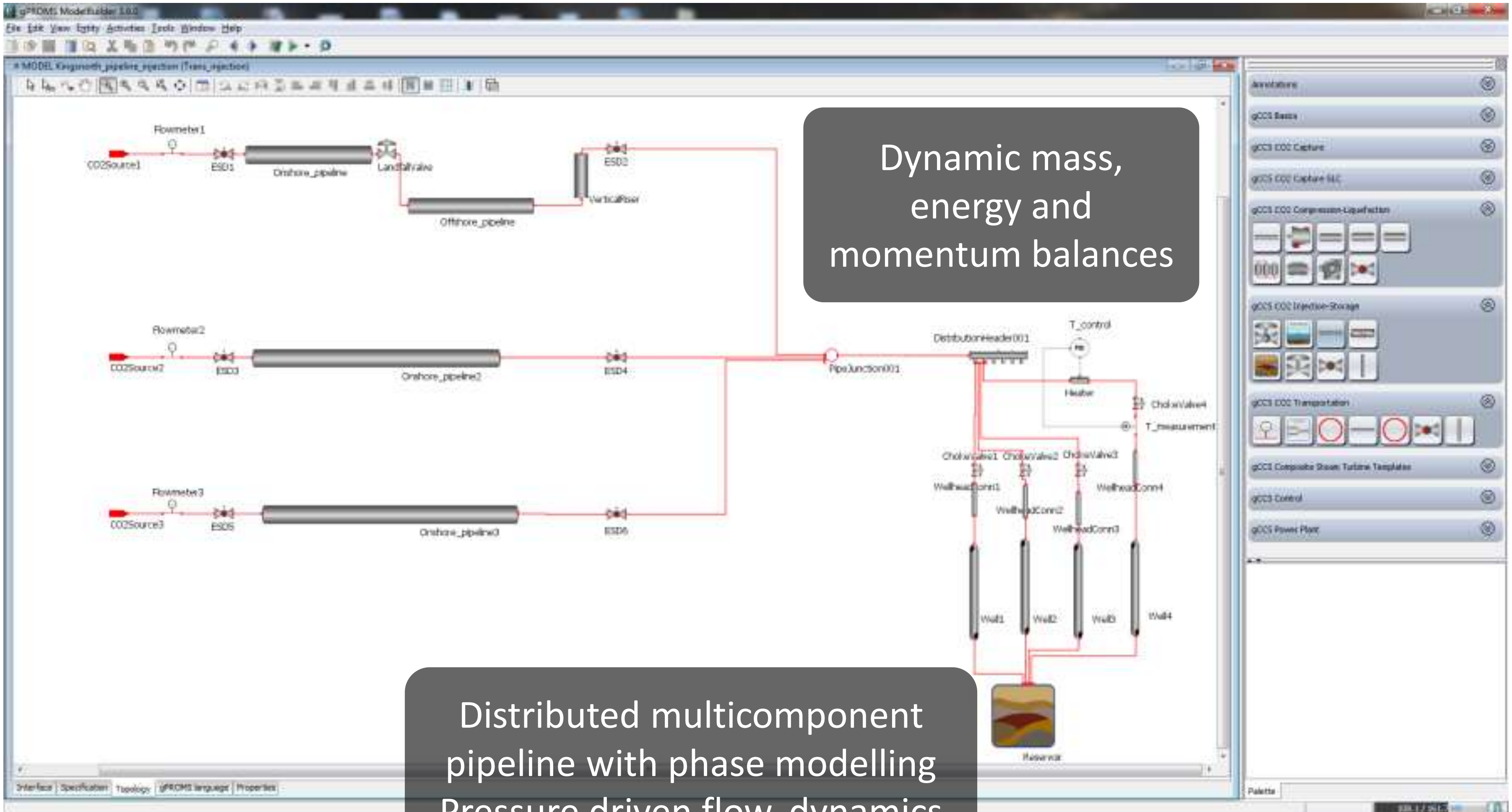
# Transmission & injection flowsheet




Dynamic mass, energy and momentum balances

Distributed multicomponent pipeline with phase modelling
Pressure driven flow, dynamics
Heat to/from environment

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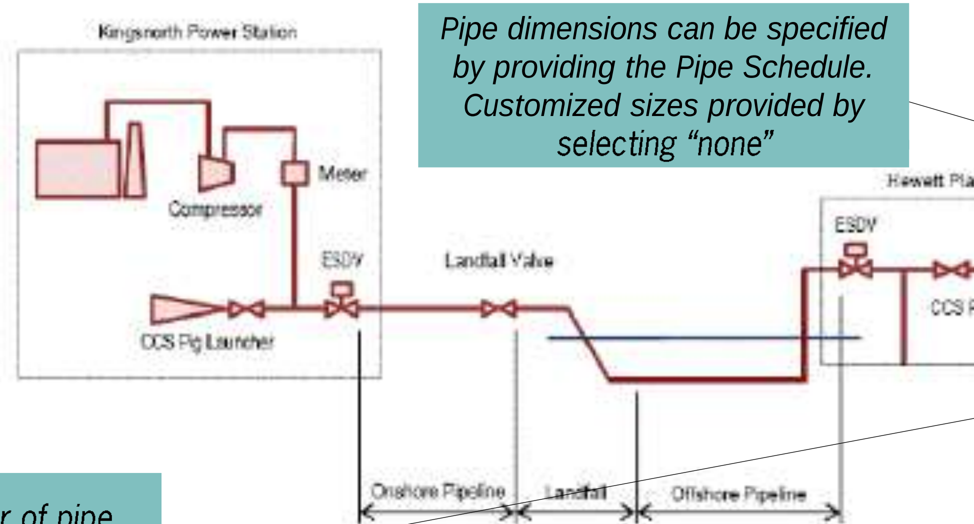
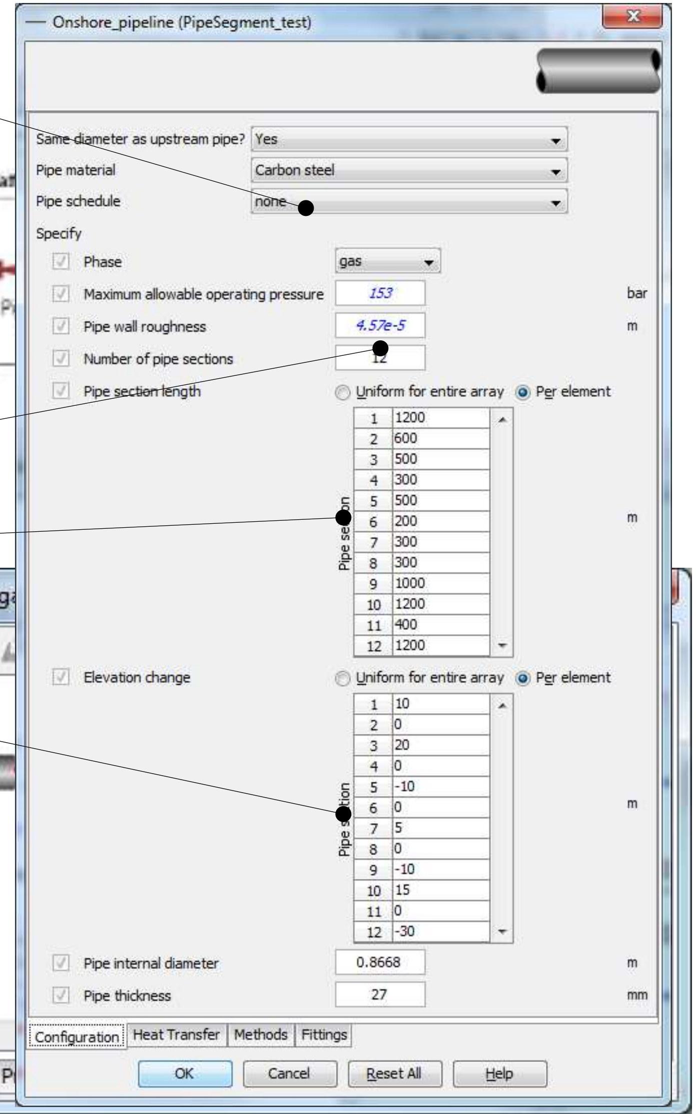
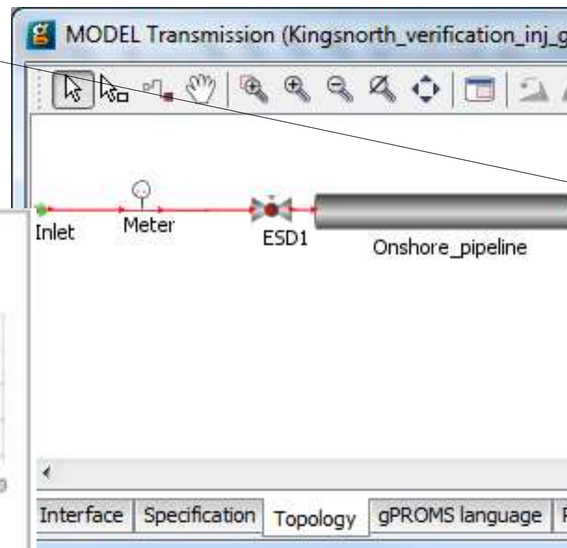
# Transmission System – Example: Kingsnorth FEED Onshore Pipeline

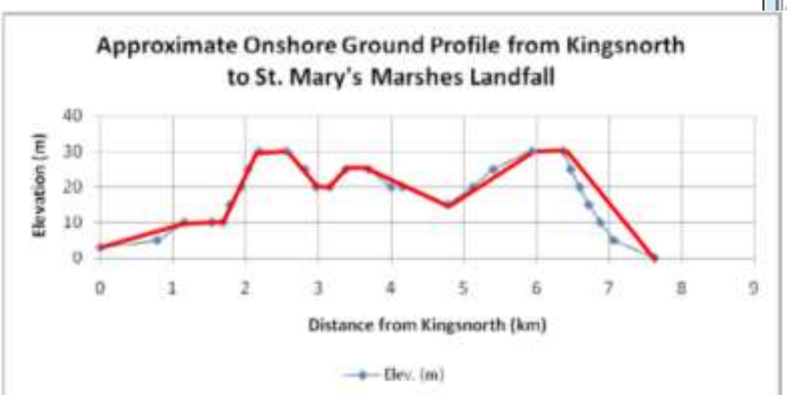
*Pipe dimensions can be specified by providing the Pipe Schedule. Customized sizes provided by selecting "none"*




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



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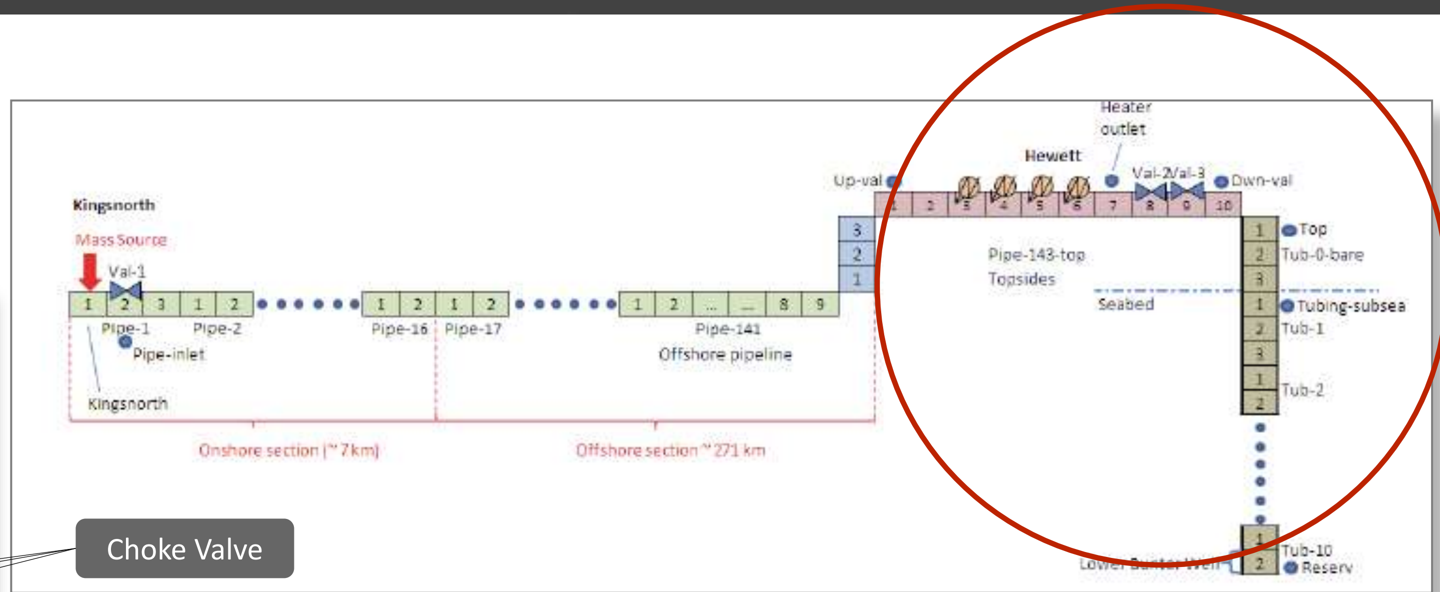
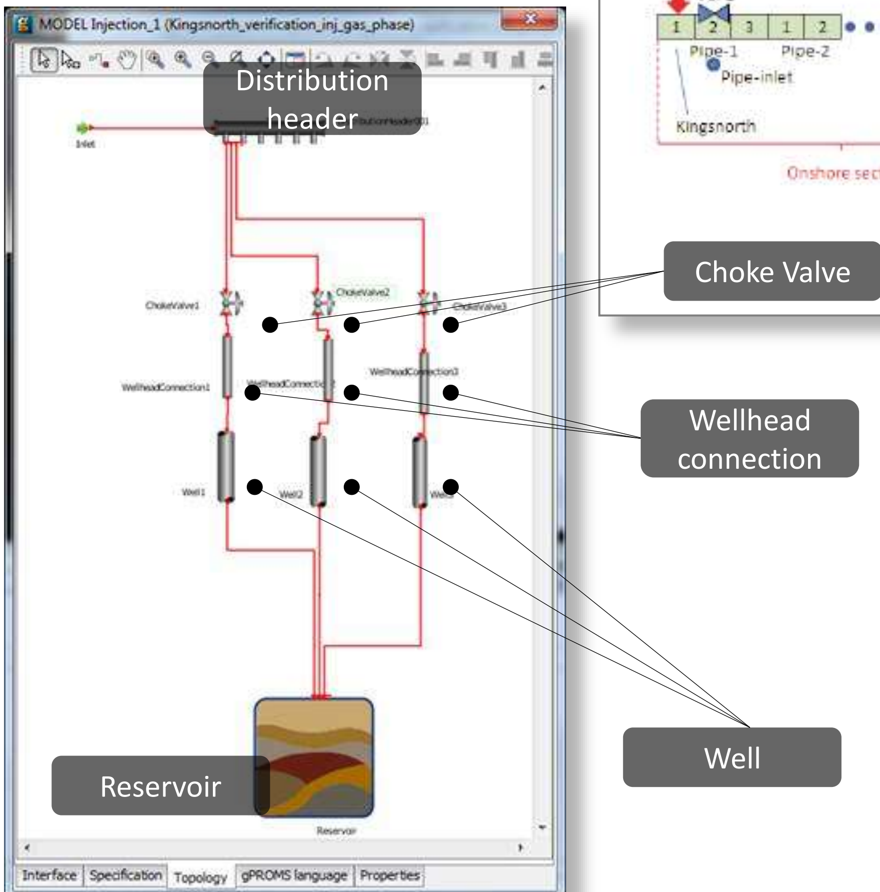
# Tool-kit components

## Model libraries – $CO_2$ Transmission and Injection/Storage

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



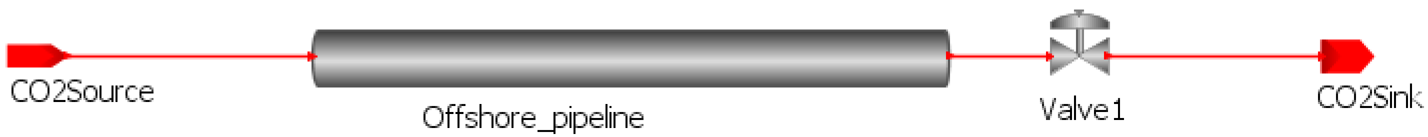




| For gas phase operation (reservoir pressure 2.1barg) | Kingsnorth | gCCS | % Error (abs K for temps) |
|---|---|---|---|
| ΔP between Reservoir and Bottomhole (bar) | 5.4 | 5.36 | ~0.6 |
| ΔP between Bottomhole and downstream the choke valve (bar) | 13.3 | 13.3 | ~0 |
| Fluid temperature at Bottomhole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

# Tool-kit components

Model libraries – $CO_2$ Transmission and Injection/Storage

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

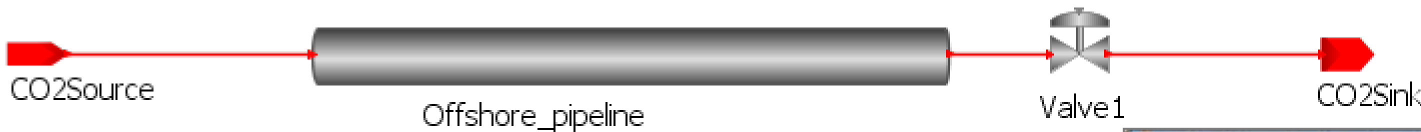


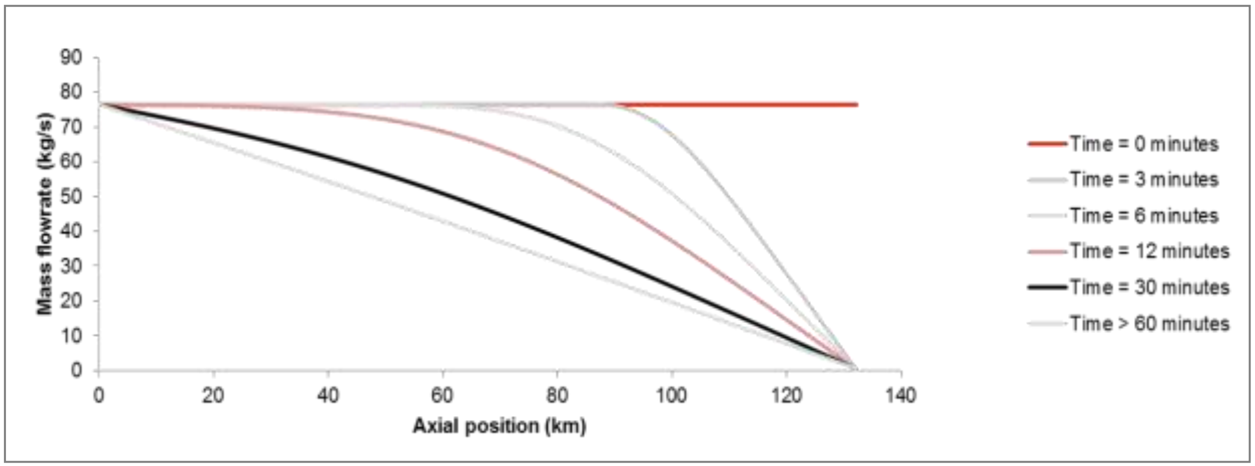

- Assumed constant inlet flowrate at CO2Source (275tonnes $CO_2$ per day)
- Gas phase injection with discharge pressure in CO2 sink ~ 21bara
- Total pipeline length – 132.2km
- Pipeline is located offshore (in water)

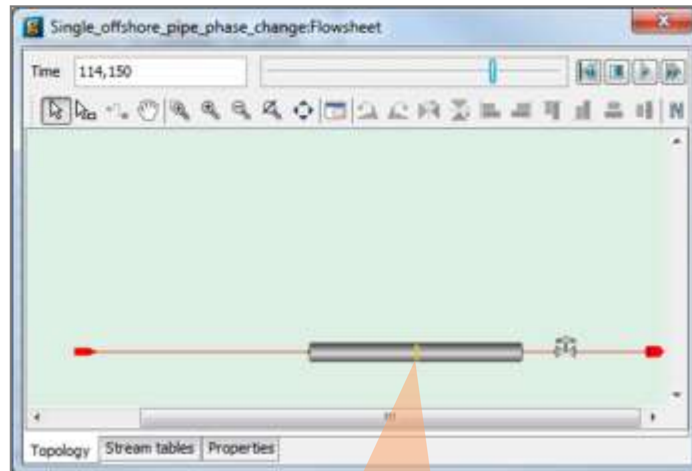
# Tool-kit components

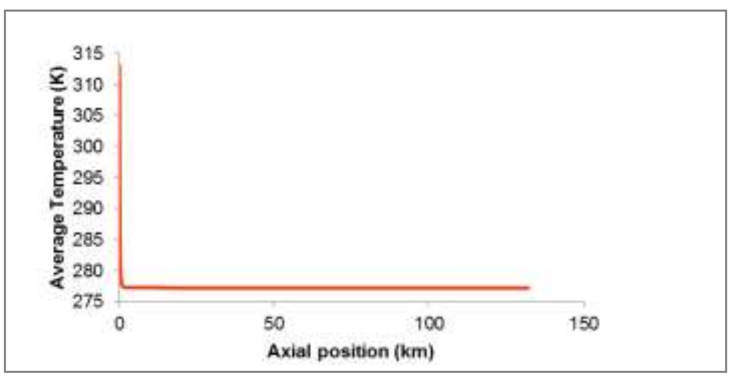
## Model libraries – $CO_2$ Transmission and Injection/Storage

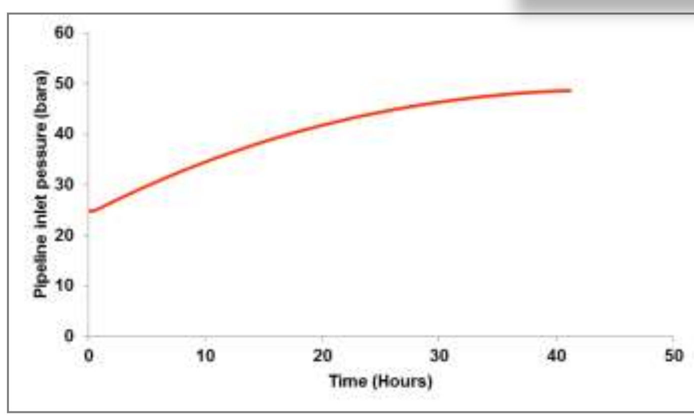
- System dynamics
  - Simulating **line-packing operation**: Sudden valve closure




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

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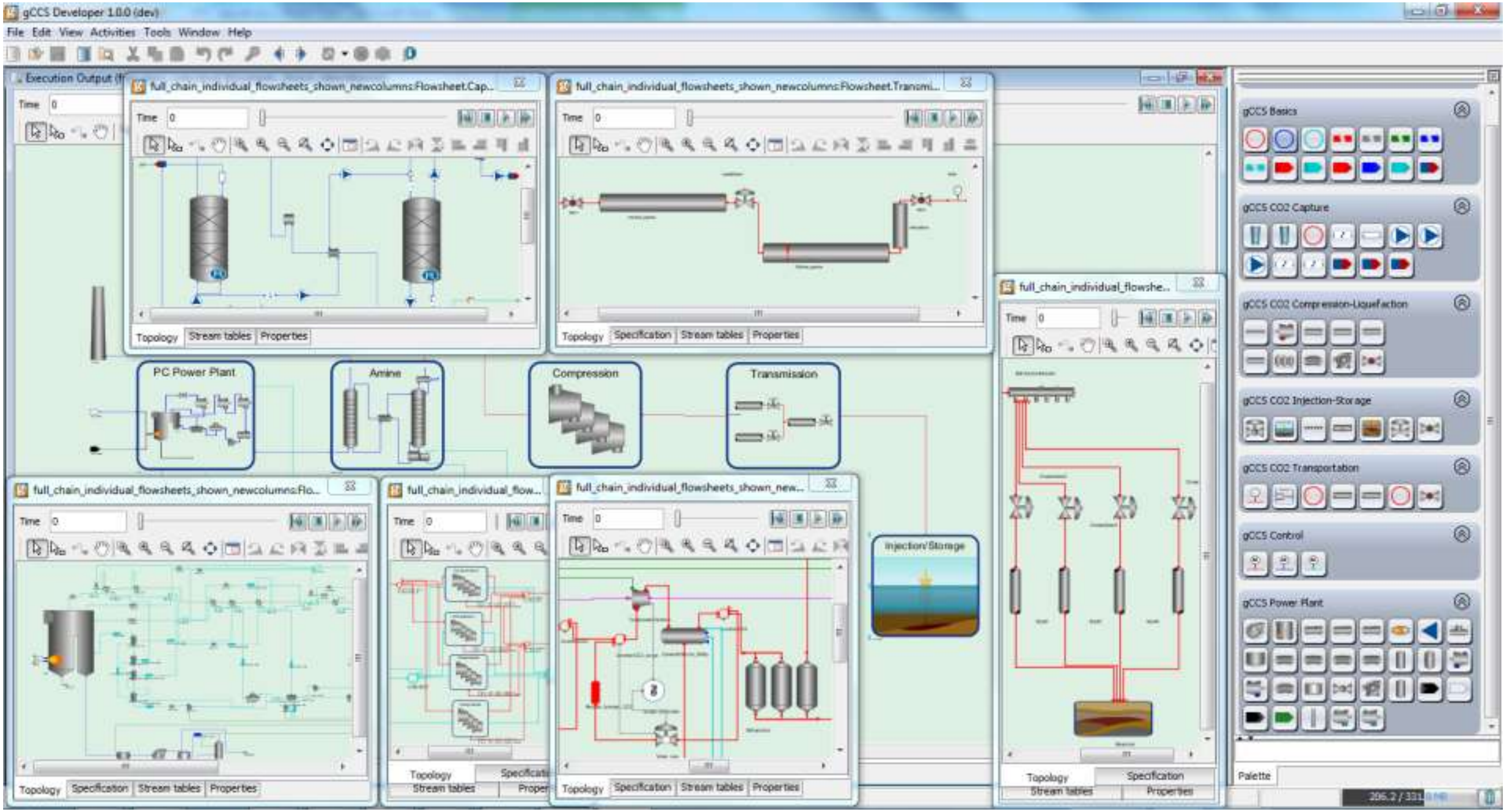
# Tool-kit components

## Whole-chain simulation

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

# Challenges

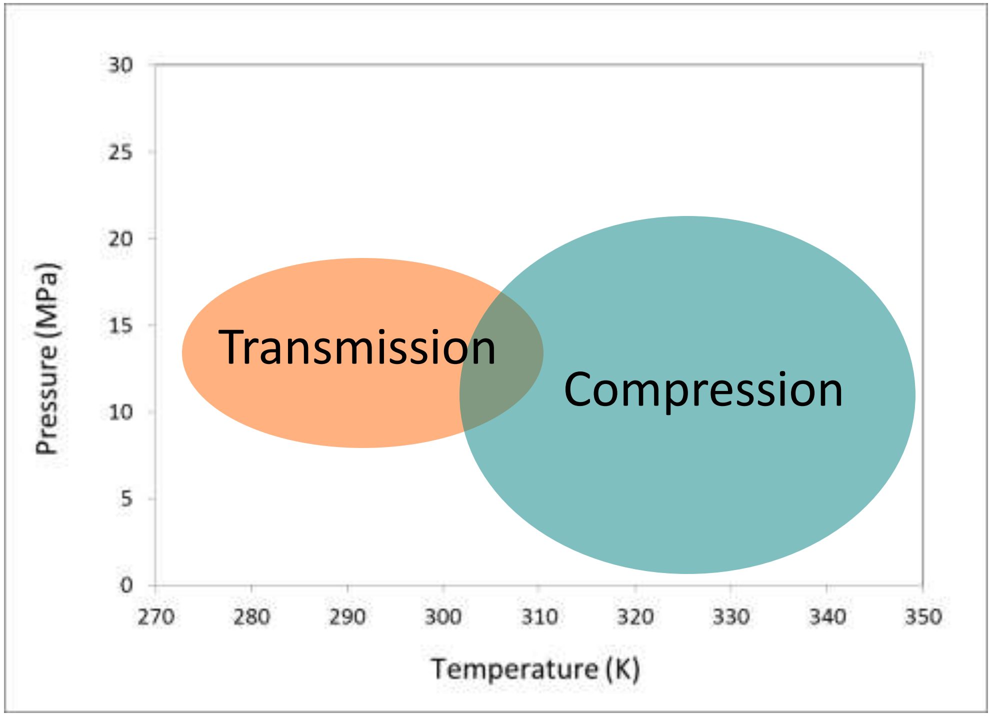
- Impurities
- Wide range of conditions
- Limited experimental data

→ A predictive equation of state is required

- applied to mixtures of $CO_2$, CO, $H_2O$, Ar.....
- small molecules → single group each

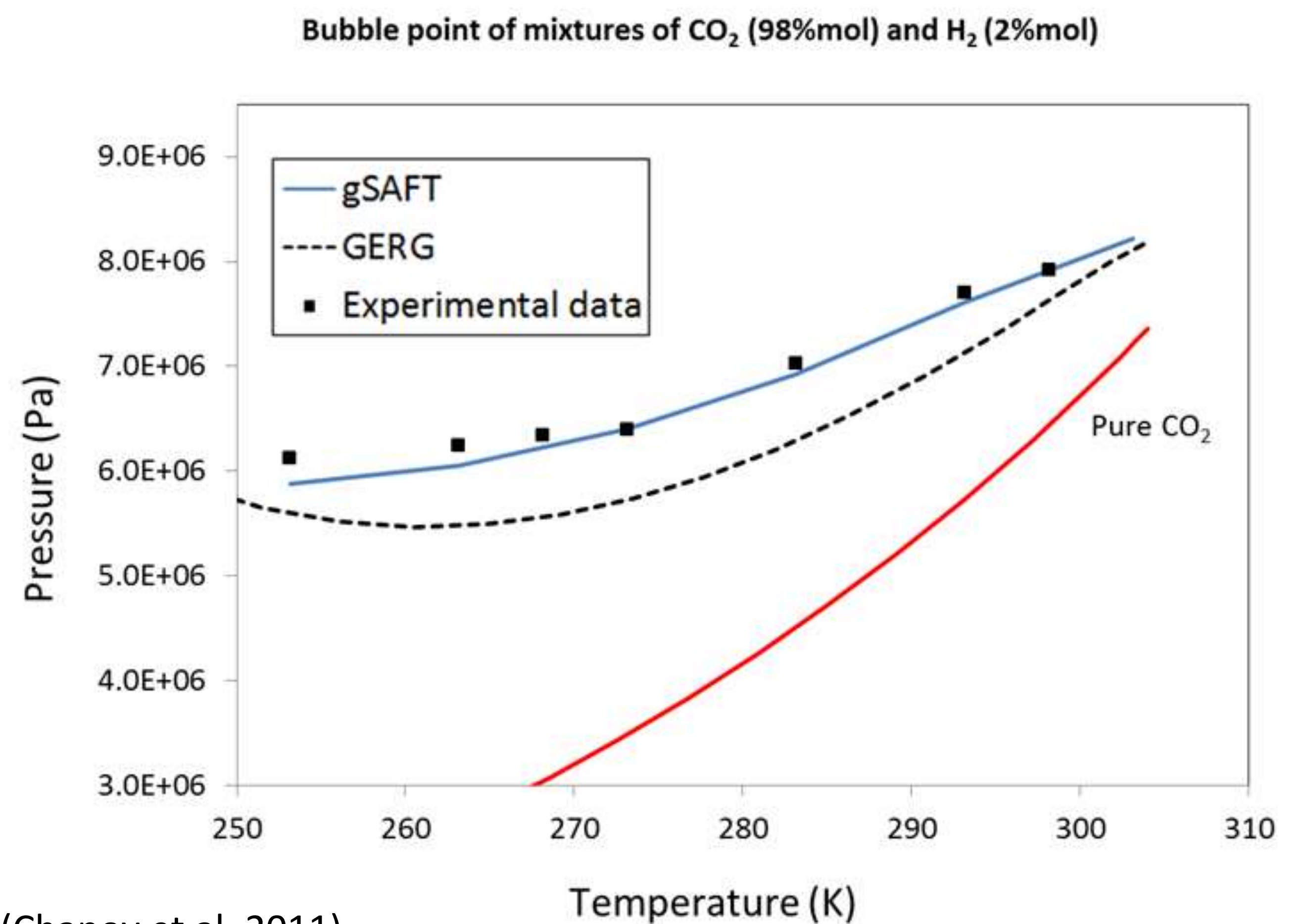
# Challenges II: Wide range of conditions

- Compression subsystem
  - Pressures
    - Inlet 0.5 to 5 bara
    - Outlet 10 to 200 bara
  - Temperatures
    - Inlet 20-41 °C
    - Outlet 40-130 °C
- Transmission subsystem
  - Pressures
    - 50-200 bara
  - Temperatures
    - -5-40 °C



# 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

# 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 3$^{rd}$-party models
- **Soon** (2-4 month timescale)
  - IGCC, oxyfuel power generation
  - Capture – physical absorption
  - Integration with advanced physical properties engine (SAFT-$\gamma$ Mie)
- **To follow** (6-9 month timescale)
  - Costing
  - Project-ready environment

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# With thanks to the ETI and our partners

- *This work was carried out as part of a* £3m project commissioned and co-funded by the **Energy Technologies Institute** (ETI) and project participants **E.ON**, **EDF**, **Rolls-Royce**, **Petrofac** (via subsidiary **CO2DeepStore**), **PSE** and **E4tech**.

- The project is aimed at delivering a robust, fully integrated tool-kit that can be used by CCS stakeholders across the whole CCS chain.

# PSE's CCS Tech Team

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  - Compression Systems
  - Capture processes
- Dr Adekola Lawal
  - Capture processes
  - Transmission & injection
- Dr Javier Rodríguez
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  - Physical properties (gSAFT)
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  - Product development
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  - Software development
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# Thank you!

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