The key role of modelling from R&D to Design and Operation

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Reserves: Our use of the term "reserves" in this presentation means SEC proved oil and gas reserves.

Resources: Our use of the term "resources" in this presentation includes quantities of oil and gas not yet classified as SEC proved oil and gas reserves. Resources are consistent with the Society of Petroleum Engineers 2P and 2C definitions.

Organic: Our use of the term Organic includes SEC proved oil and gas reserves excluding changes resulting from acquisitions, divestments and year-average pricing impact.

Resources plays: Our use of the term 'resources plays' refers to tight, shale and coal bed methane oil and gas acreage.

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Outline

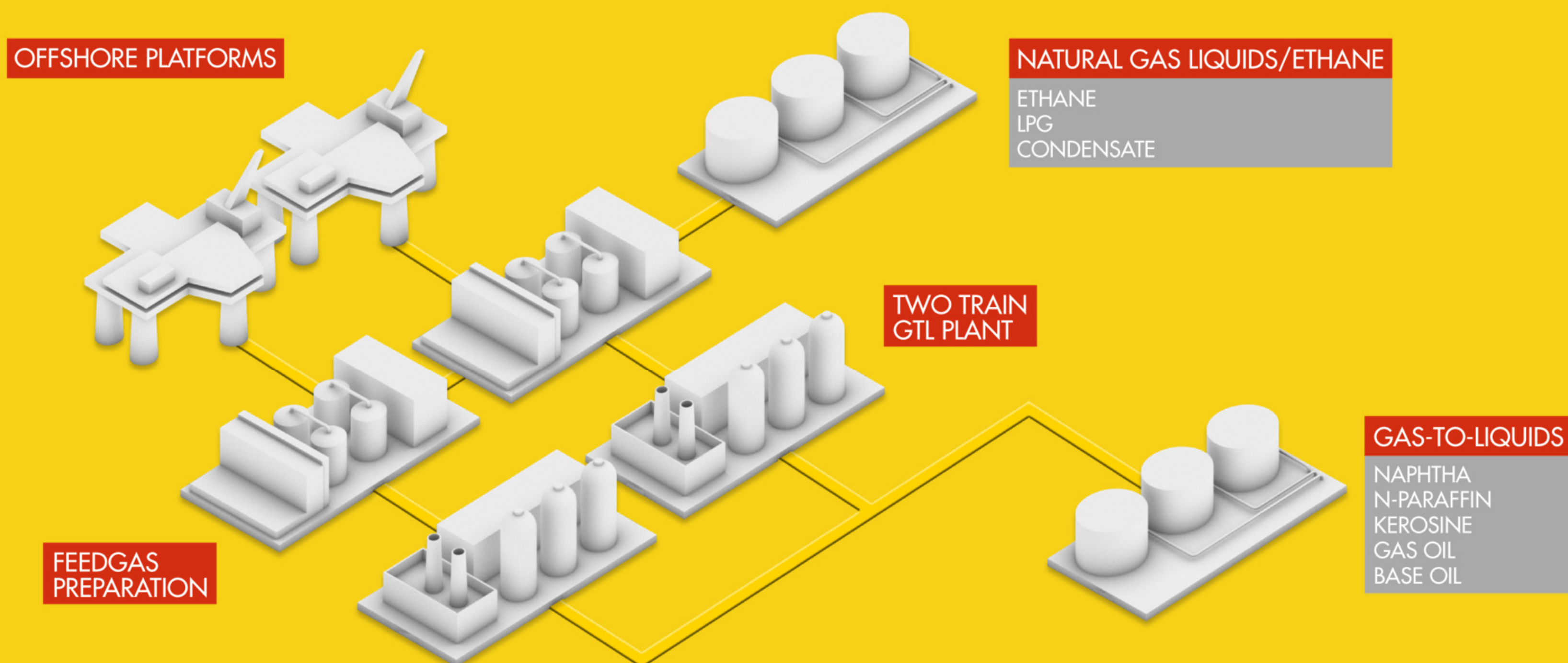
- Gas-To-Liquids and its Innovation Cycle
- Advanced Process Modelling for GTL: an overview
- Heavy Paraffin Synthesis Reactor Model
- APM Case Studies
- Summary and Conclusion

1

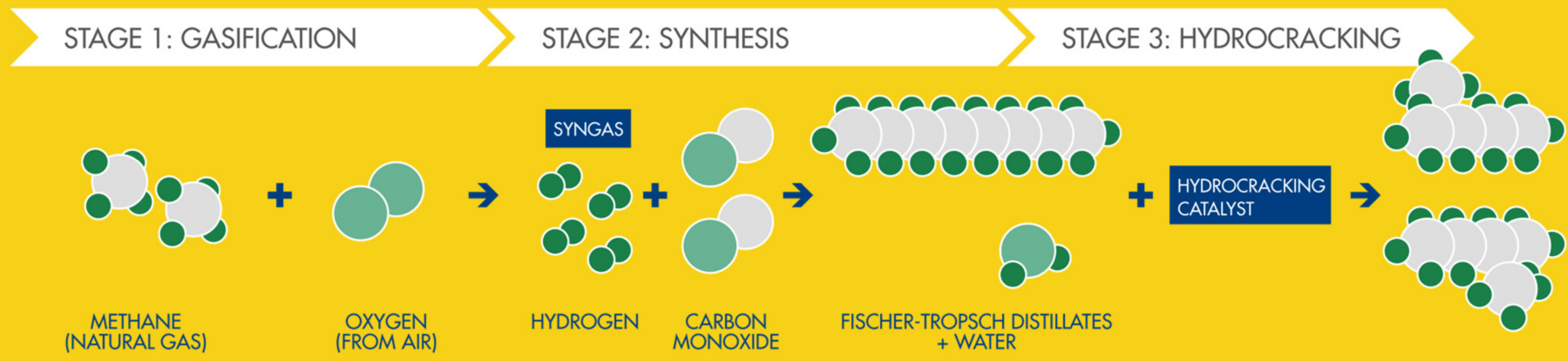
GTL and its Innovation Cycle

PEARL GTL - INTEGRATED GAS-TO-LIQUIDS PROJECT

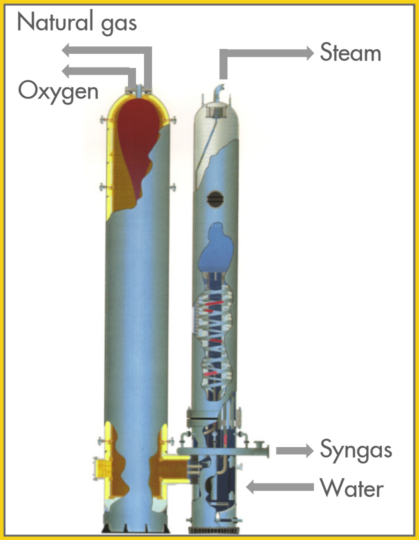
- 1.6 Bcf/d of Wet Gas
- 120 kbbl/d Ethane/NGLs
- 140 kbbl/d GTL products
- Full integration from offshore to refined products
- In production since mid 2011



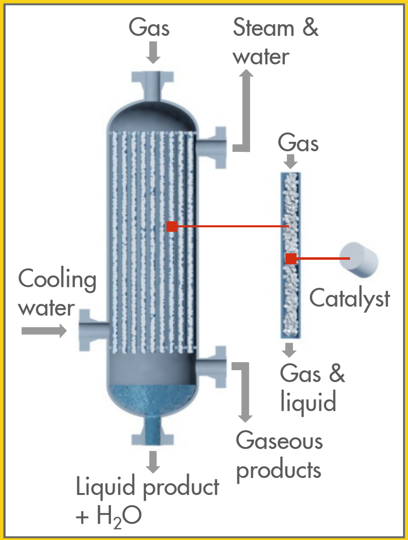
PEARL GTL - TECHNOLOGY FUNDAMENTALS



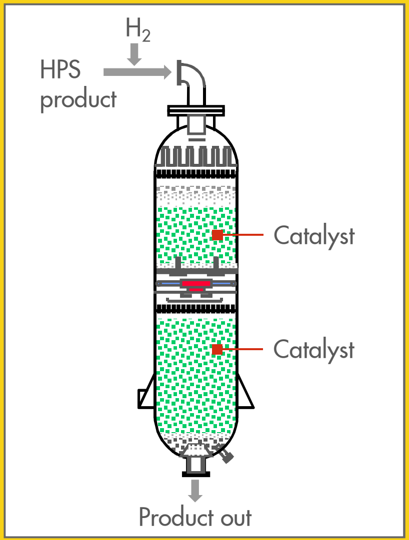
PEARL GTL - TECHNOLOGY FUNDAMENTALS



- Shell Gasifications Process (SGP) based on Partial Oxidation (POX)
- 18 SGPs
- Reaction temperature: ~ 1300 °C
- Refractory clad reactor



- Heavy Paraffin Synthesis (HPS)
- 24 reactors of 1,200 tonnes each
- 10's of thousands of tubes



- Heavy Paraffin Conversion (HPC)
- Largest hydrocracker in Shell
- Catalyst dedicated to GTL
- Maximizing yield of gasoil and BO

GTL: A 40 YEAR JOURNEY OF TECHNOLOGY AND PRODUCT INNOVATION

1973

- Laboratory Amsterdam
  grams/d

1983

- Pilot plant Amsterdam
  3 bbl/d

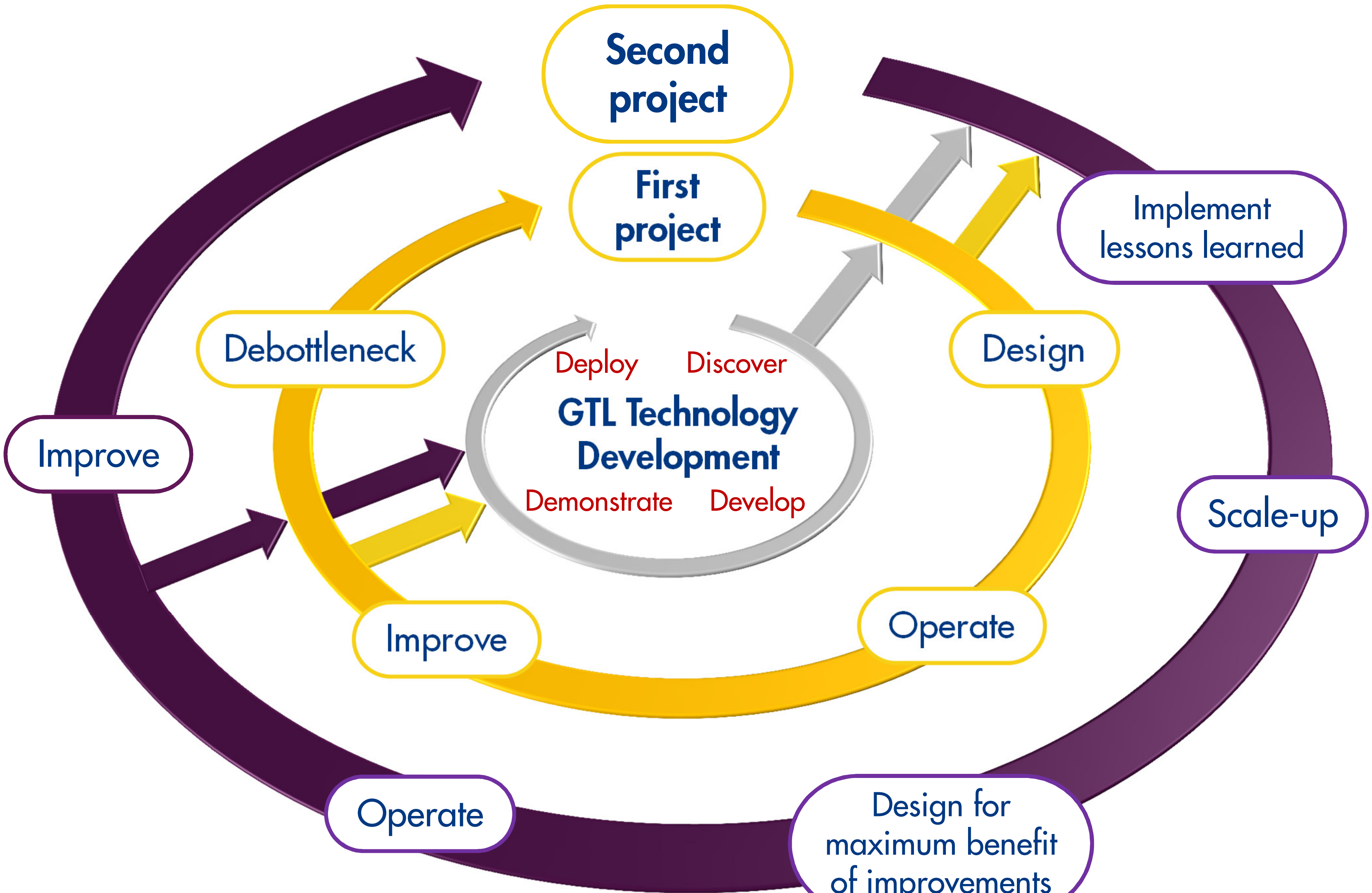
1993

- Bintulu Malaysia
  current capacity
  14,700 bbl/d

TODAY

- Pearl GTL Qatar
  140,000 bbl/d

INNOVATION CYCLE FOR GTL TECHNOLOGY DEVELOPMENT



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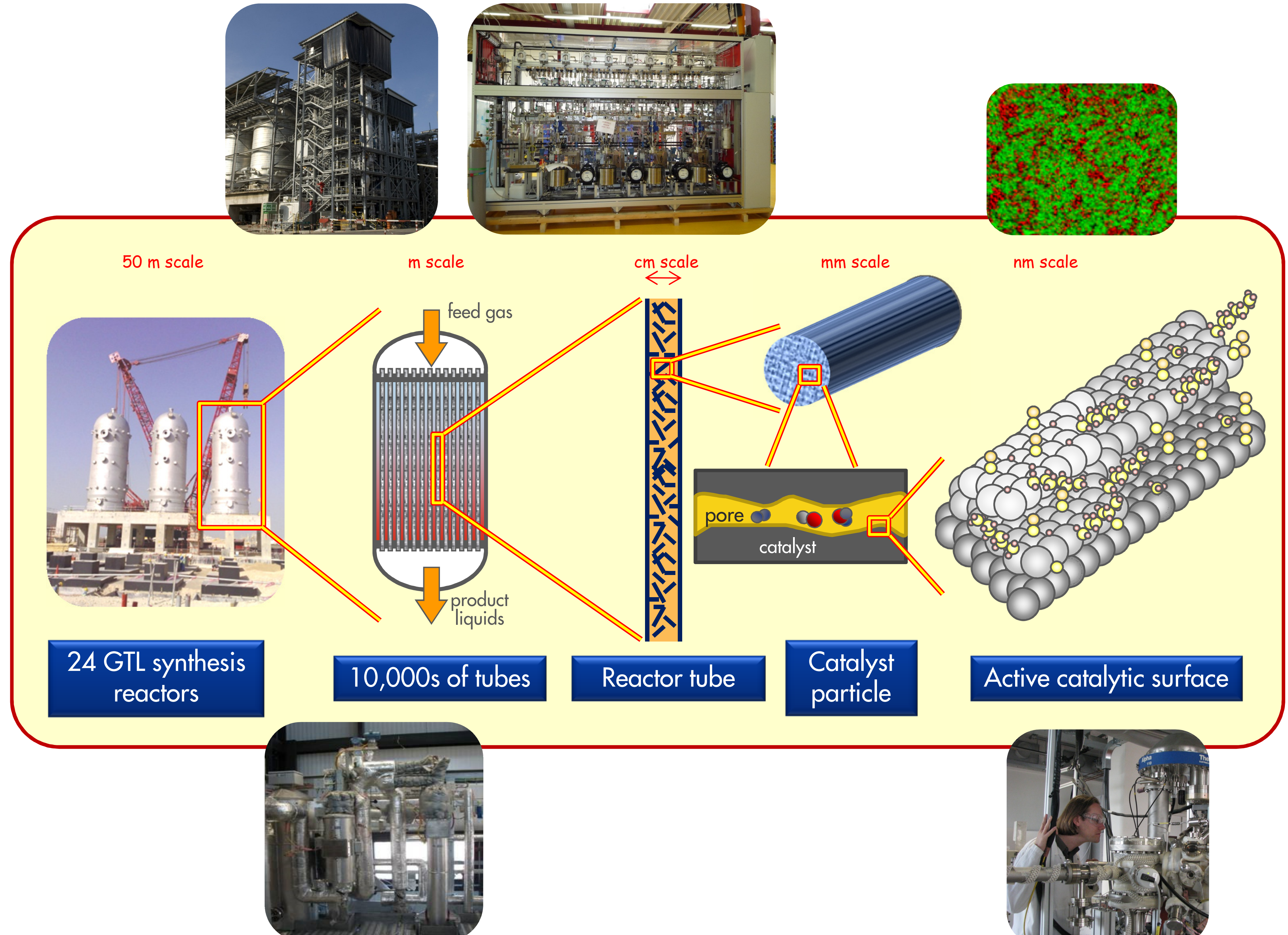
Advanced Process Modelling for GTL: an overview

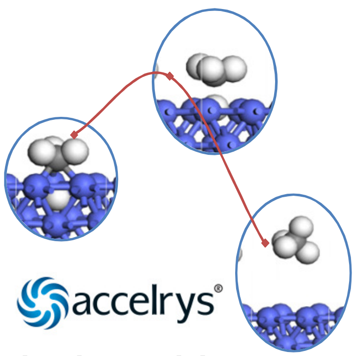

50 m scale
m scale
cm scale
mm scale
nm scale
feed gas
product liquids
pore
catalyst
24 GTL synthesis reactors
10,000s of tubes
Reactor tube
Catalyst particle
Active catalytic surface

MULTI-SCALE MODELING FOR GTL: FROM CATALYST SURFACE….

Explanatory R&D:
What is happening at the surface?

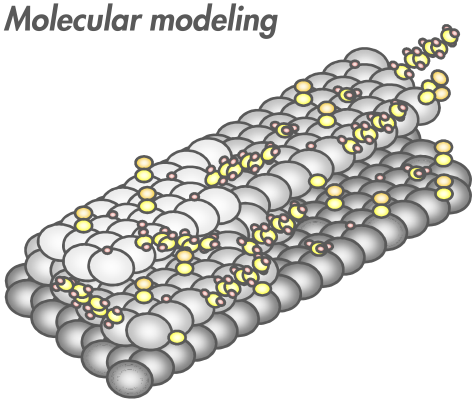
Exploratory R&D:
New catalyst formulations:
higher productivity – selectivity - stability

Novel catalyst – reactor systems
Lower capital intensity - higher carbon efficiency

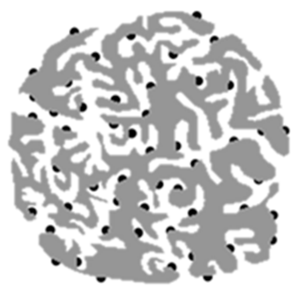


accelrys®

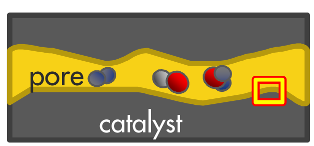
Molecular modeling



… and inside the pores (mass transfer modeling)



5 - 100 nm scale



mm scale

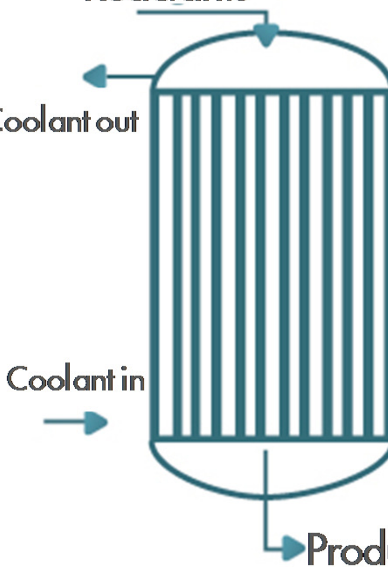
wax-filled cat pellet

… modeling of intrinsic kinetics with advanced parameter estimation techniques

gPROMS

cm scale

m scale



… modeling of interplay hydrodynamics, mass & heat transfer and reaction kinetics DAE

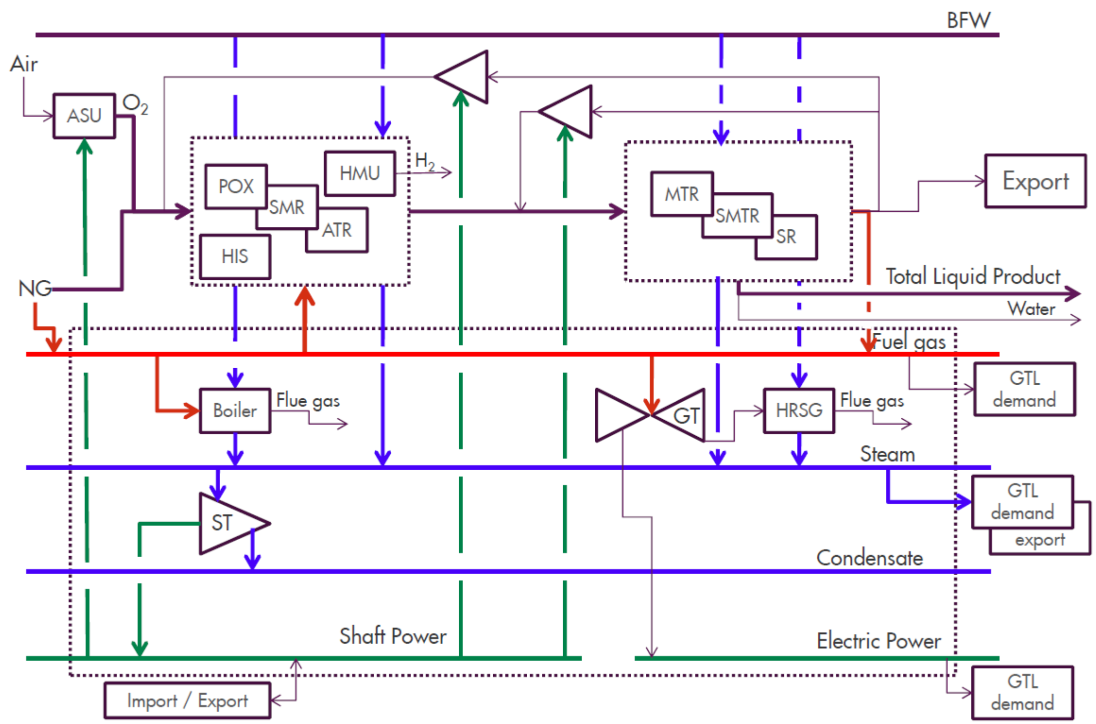
gPROMS

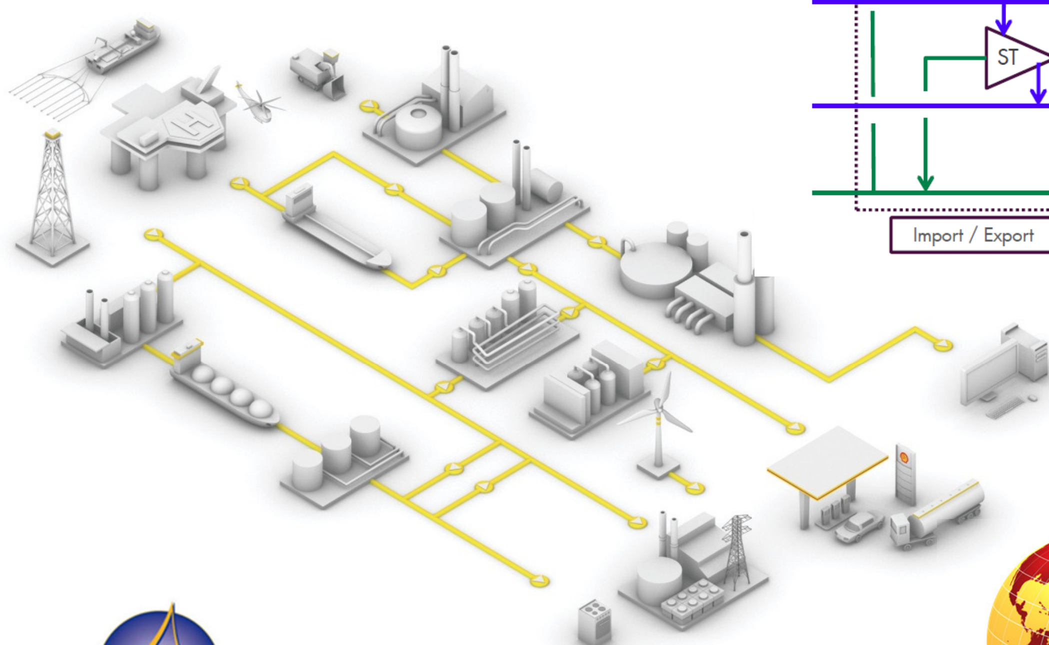
...TO THE GAS VALUE CHAIN LEVEL

Process Integration:

Lower capital intensity -
higher carbon efficiency -
higher product value

Process Synthesis Tool (MINLP)





Competitive analysis:

How does GTL compare to alternative gas monetization options: LNG, G2C, G2P ?
Used for performance target setting

Gas Value Chain Analysis Tool (MILP)

GMOS/NetSim
Decision Support System for optimizing supply chains

3

HPS Reactor Modelling

HPS REACTORS @ SMDS & PEARL

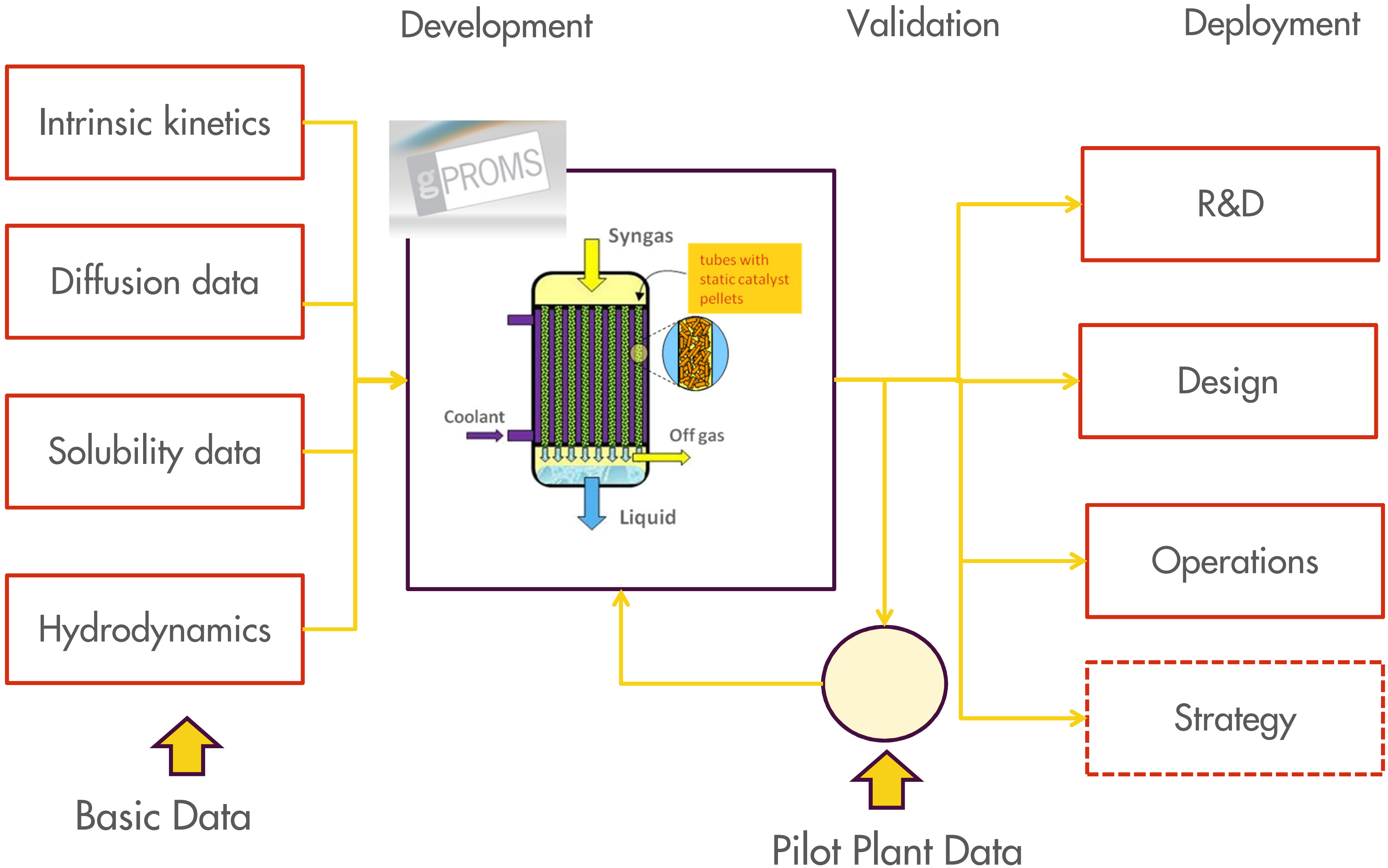
SMDS Bintulu: 4 HPS Reactors

Pearl GTL: 24 HPS Reactors

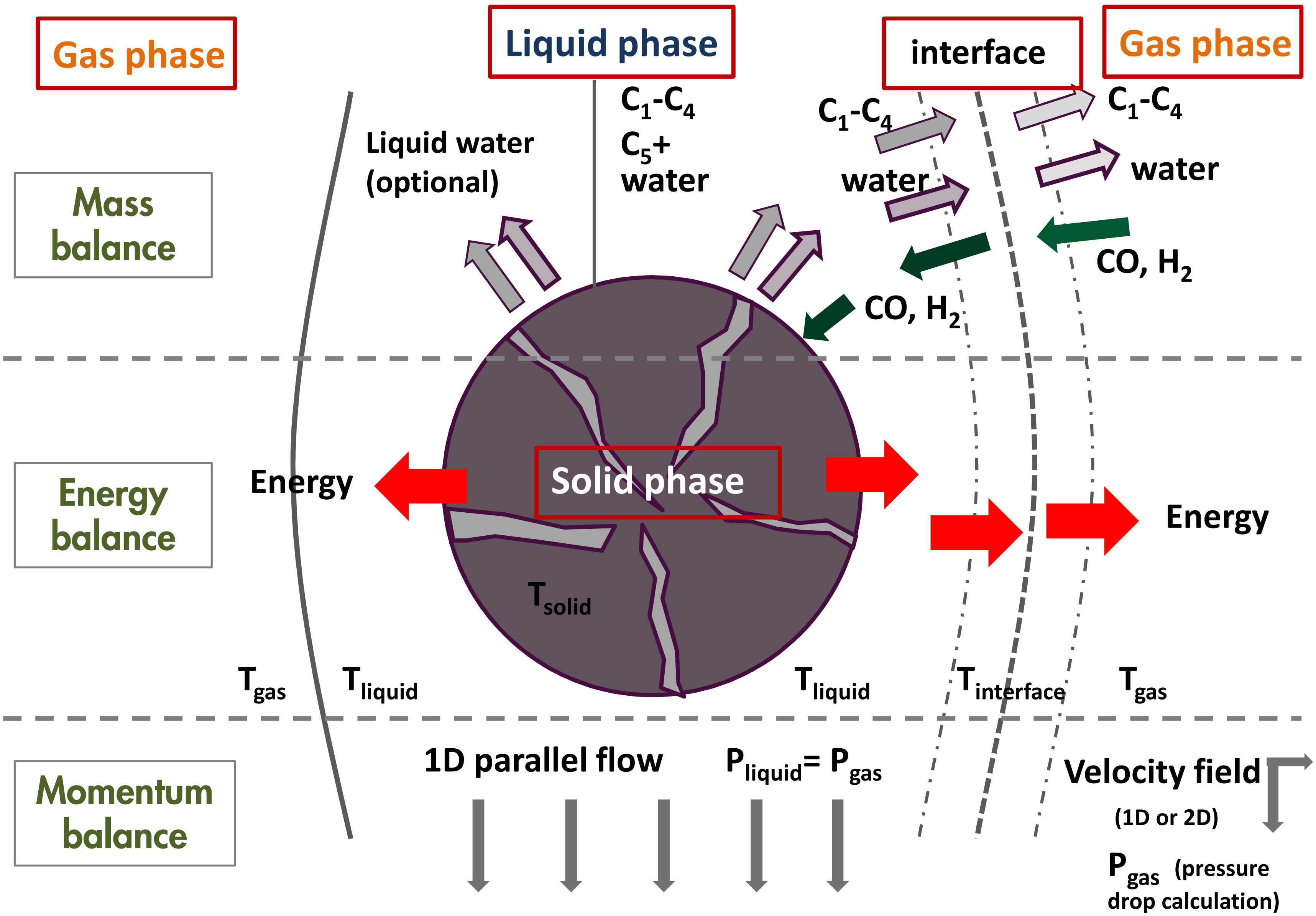
Equality principle for HPS Reactors: "All tubes to be equal, in terms of:"

- flow per tube
- conversion per tube
- stability per tube

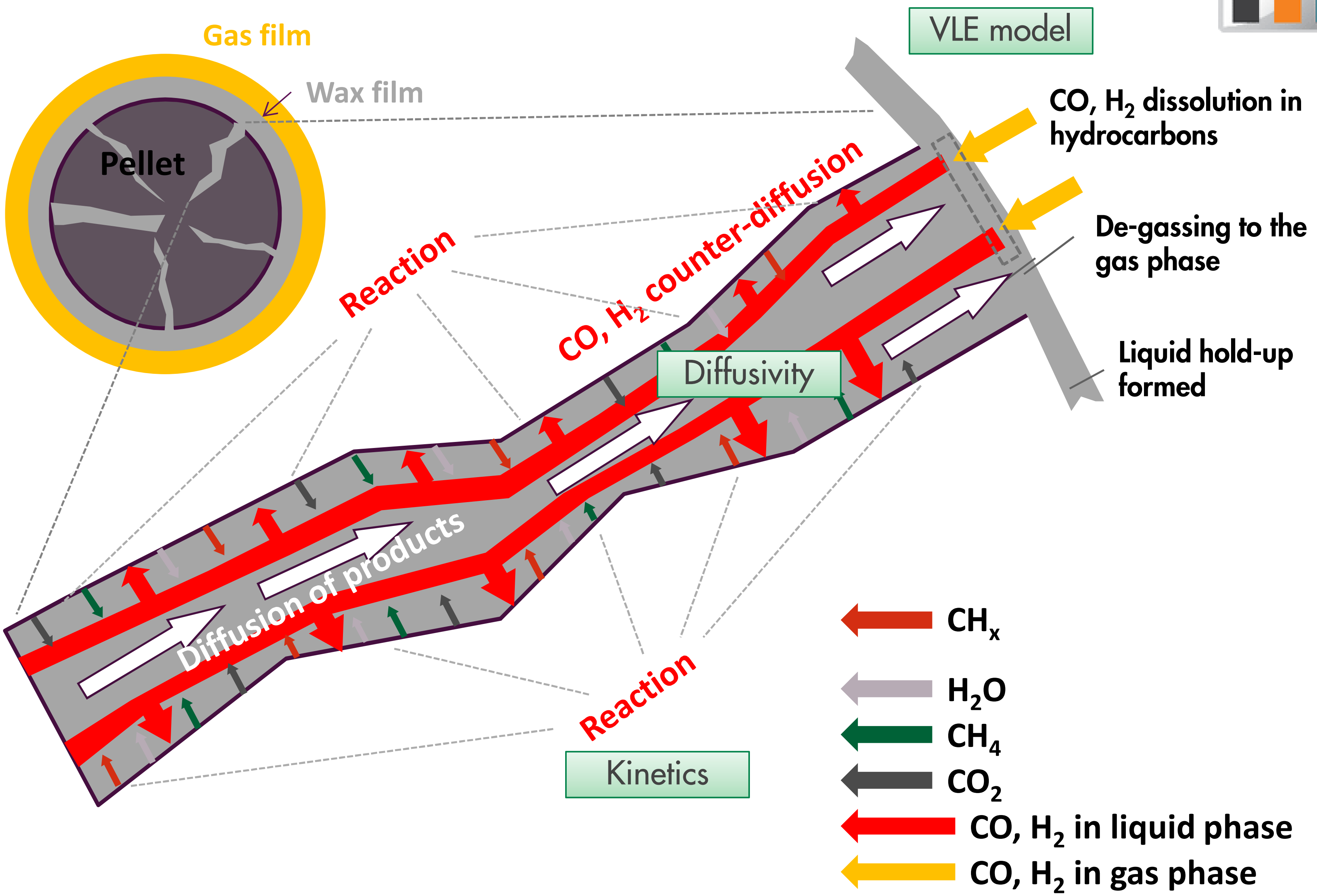
HPS REACTOR MODEL DEVELOPMENT & DEPLOYMENT



MODELLING DETAILS AT CATALYST PELLET LEVEL

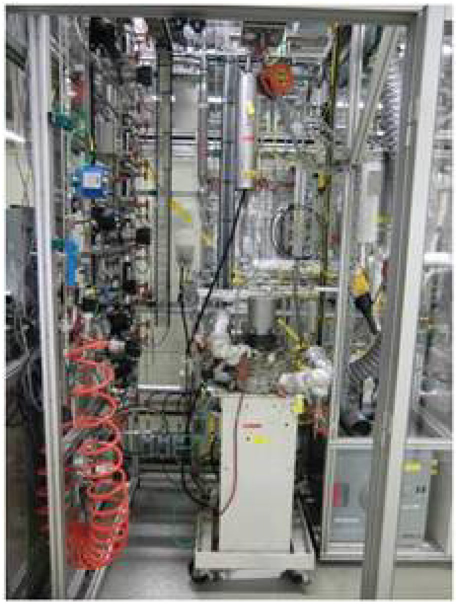


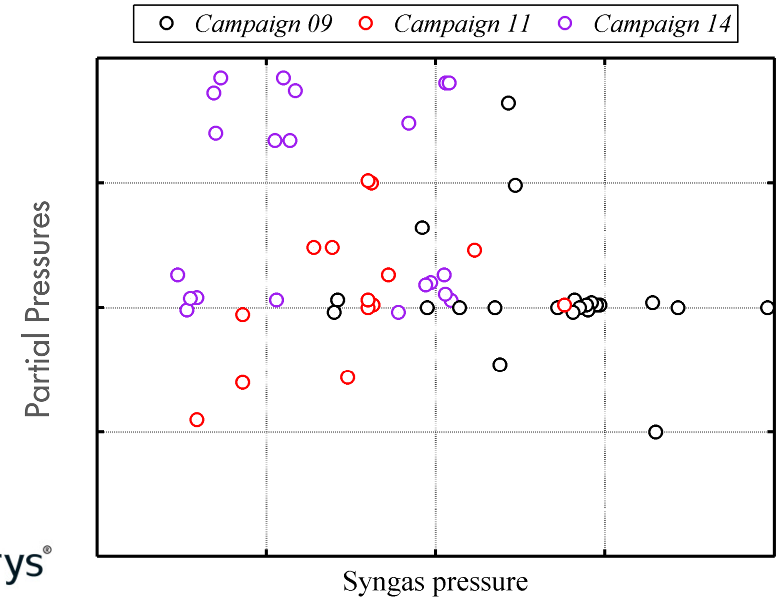
INSIDE THE CATALYST PELLET



INTRINSIC KINETIC MODEL

- Experimental campaigns → Basic data for intrinsic kinetic model
- Validity window limited to experimental window: only interpolation allowed



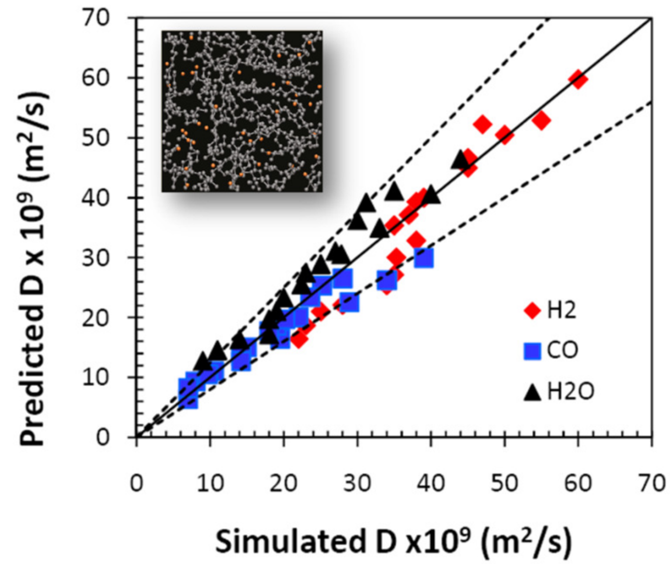


- Micro kinetic modelling (molecular modelling) to explore operating conditions beyond this window:
  - Start from given morphology of the active phase
  - Compute thermodynamic data and kinetic parameters for single reactions
  - Build a micro-kinetic model (respecting morphology) & explore wider window
  - Carry out validation experiments to confirm interesting operating conditions

DIFFUSION OF H2, CO AND H2O IN LIQUID WAX

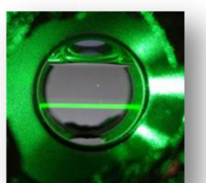
Measuring diffusion data at relevant conditions is challenging:

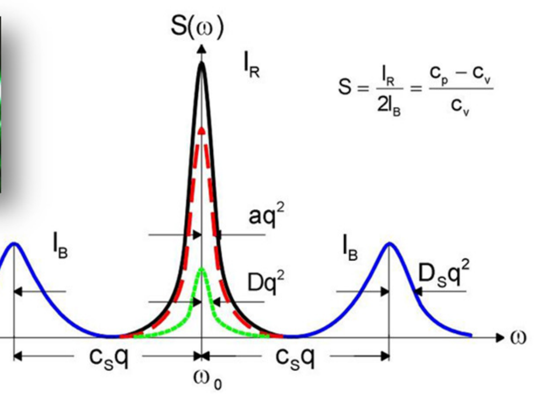
- High Performance Computing
  - Application of Molecular Dynamics
- Experimental data
  - Dynamic Light Scattering
  - Validate theoretical methods



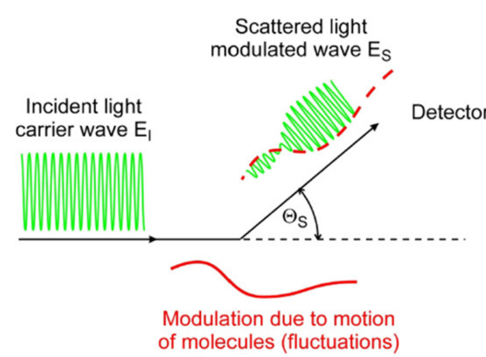
Spectrum of Scattered Light

caused by local statistical fluctuations of temperature, concentration, and pressure in thermodynamic equilibrium



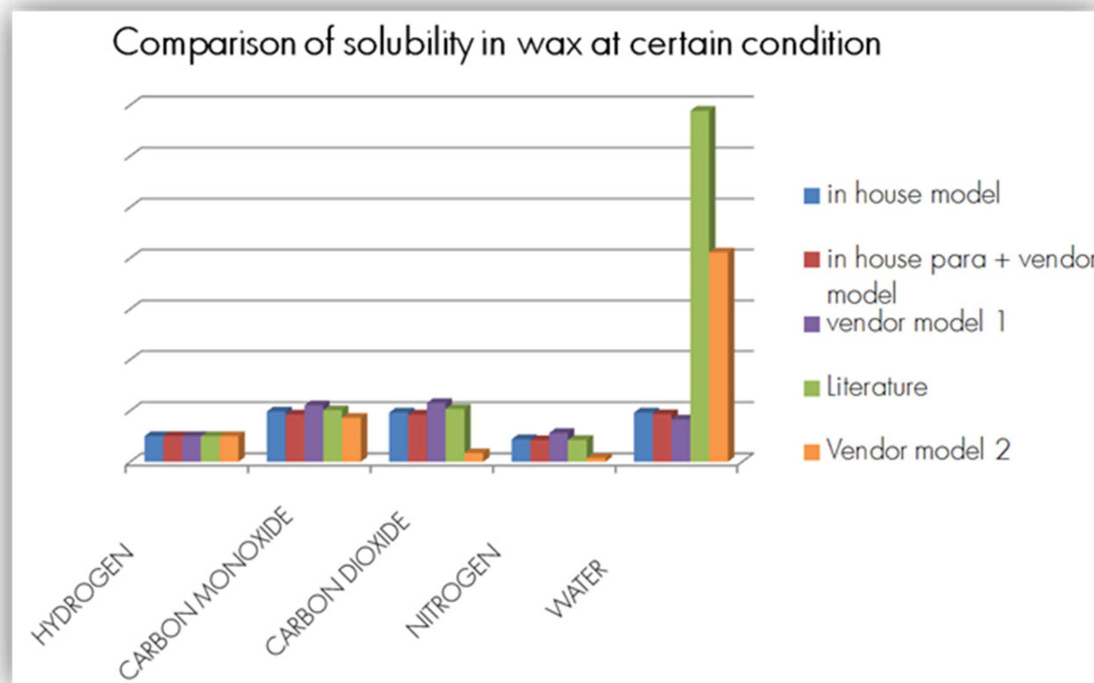


(a: thermal diffusivity; D: diffusion coefficient; c_S: sound velocity; D_S: sound attenuation; S: Landau-Placzek ratio)



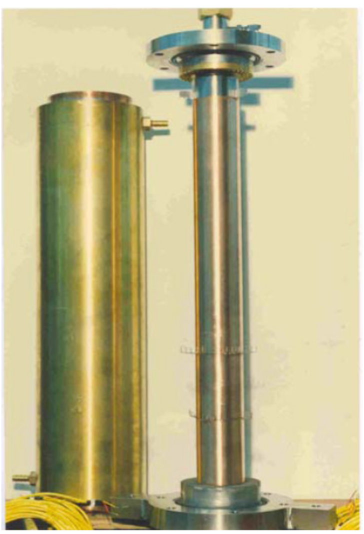
SOLUBILITY OF H2, CO AND H2O IN LIQUID WAX

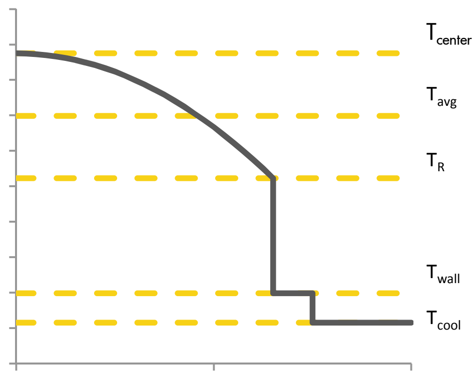
- Wax modelled as mixture of n-alkanes
- Vapour Liquid Equilibria descriptions:
  - Equation of State
  - Activity Coefficients
  - Cross checked against literature data: Dortmund Data Bank
- Temperature dependency of solubility
- Shell thermo-model ("flash engine") to be integrated with gPROMS through CAPE-OPEN

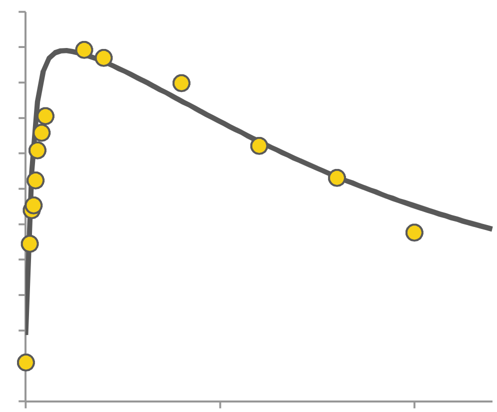


HEAT TRANSFER

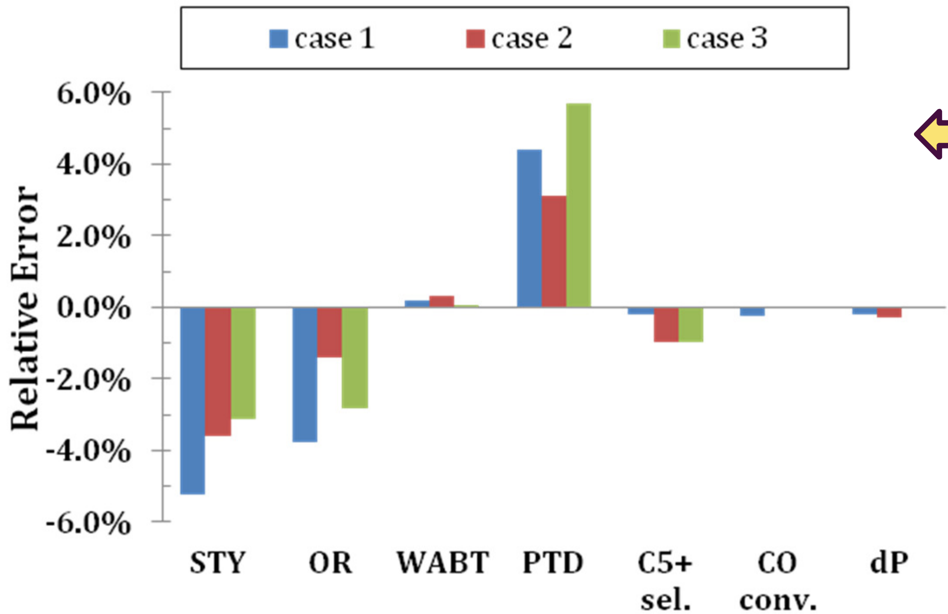
- Heat transfer coefficients for Fischer-Tropsch reactors measured in-house since 1980s using a non-reactive heat transfer cell
- Heat transfer coefficients correlated against wide set of operating conditions
- Axial and radial temperature profiles modelled in gPROMS
- Validated against measured axial temperature profiles ex HPS pilot plant:





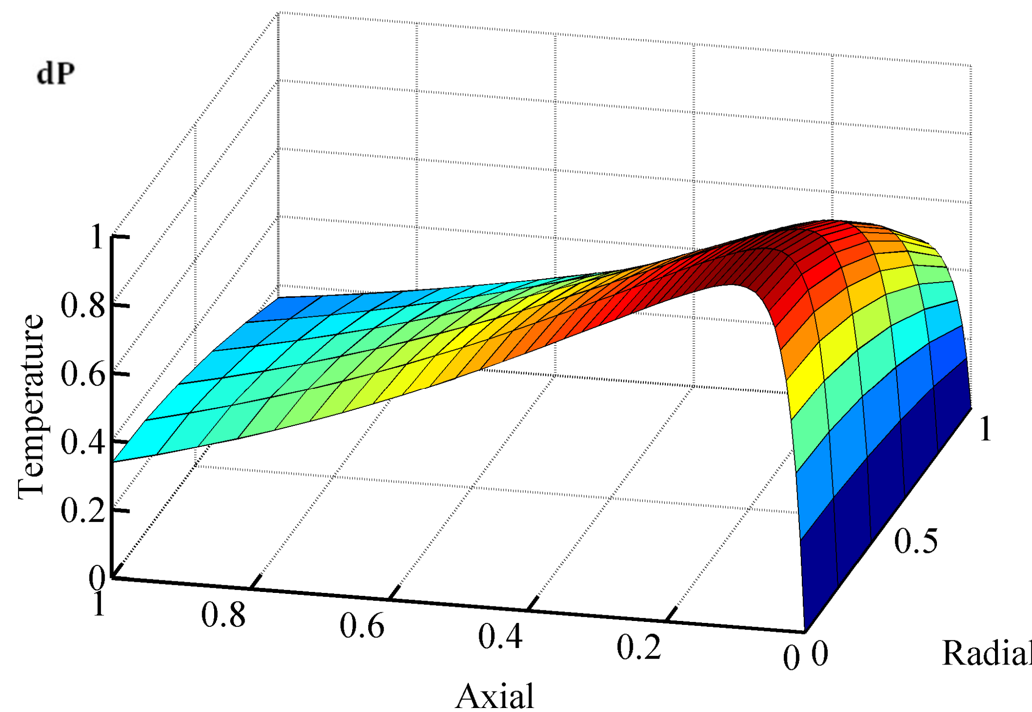


HPS REACTOR MODEL VALIDATION



Simulation results vs pilot plant data for a set of Key Performance Indicators

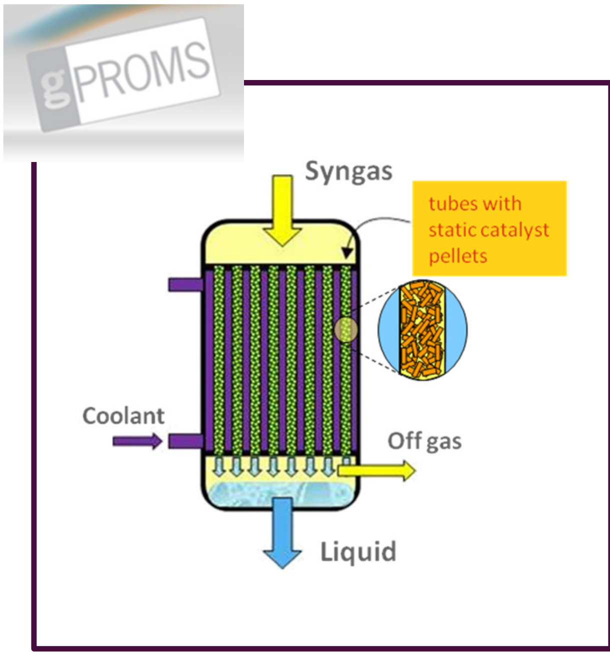
Reactor temperature profile



4

Advanced Process Modeling – Cases Studies

CASE STUDIES OVERVIEW



- R&D
  - Configuration studies
  - 1. HPS trip stability studies
- Design
  - Flowsheet Simulations
  - 2. Process Synthesis
- Operations
  - 3. APC & Optimisation
  - 4. Catalyst Deactivation
  - 5. Catalyst C/O Optimisation
- Strategy
  - 6. Gas Value Chain Studies

4.1
Trip stability studies

DYNAMIC MODELING – UPSETS IN HPS REACTORS

- Some upsets in flows may cause temperature excursions
- It is very difficult to predict whether upsets will cause a temperature excursion and if so, where in the reactor and to what extent
- Detailed dynamic reactor model in gPROMS is used to predict temperature impact upon flow upsets:

$$\varepsilon \frac{\partial \rho}{\partial t} = -\nabla(\rho\, w) \qquad \textit{continuity eq.}$$

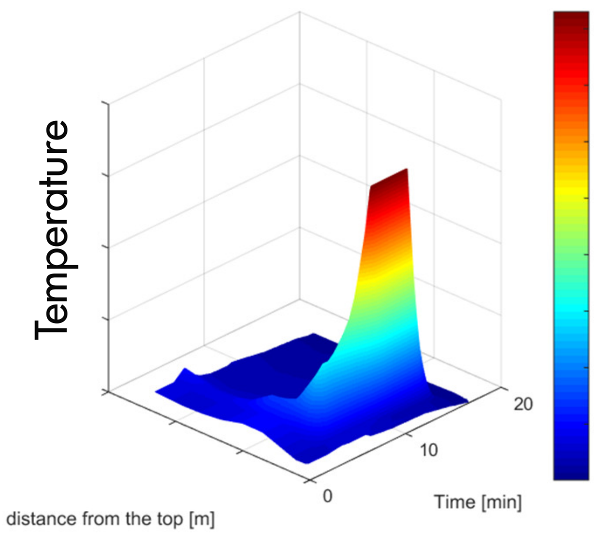
$$\varepsilon\, \frac{\partial(\rho X_i)}{\partial t} = convection + diffusion + reaction \qquad \textit{species balance}$$

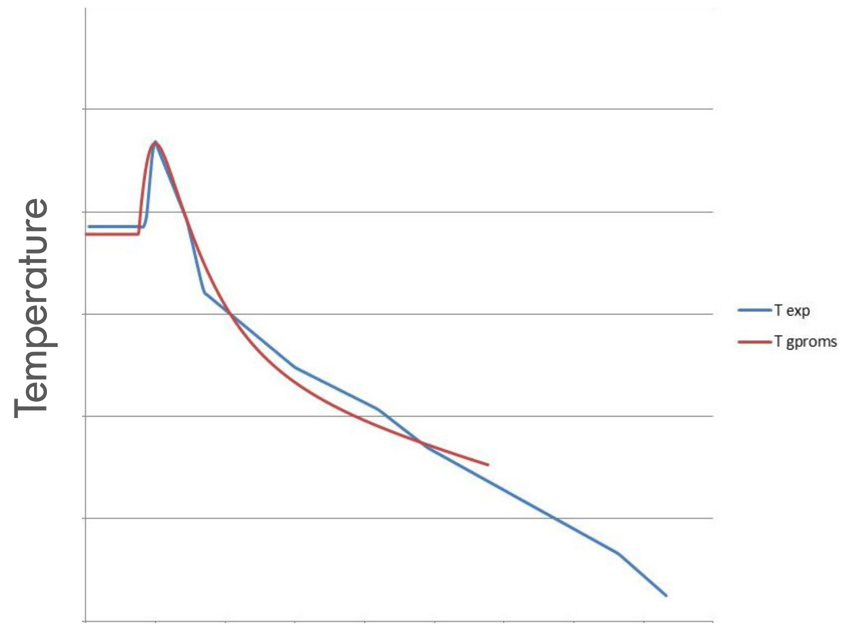
$$\varepsilon\, \frac{\partial(\rho\ cp\ T)}{\partial t} = convection + diffusion + reaction \qquad \textit{energy balance}$$

$$PV = nRT \qquad \textit{equation of state}$$

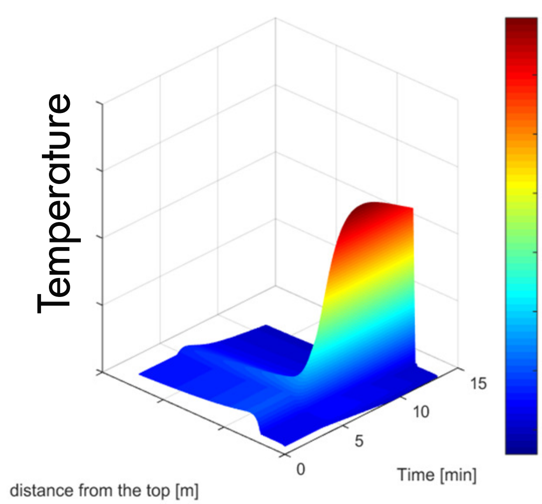
PILOT PLANT DATA VERSUS gPROMS SIMULATIONS

Experiment in the pilot plant





gPROMS simulation



gPROMS model can both qualitatively & quantitatively predict temperature excursions: when, where, to what extent

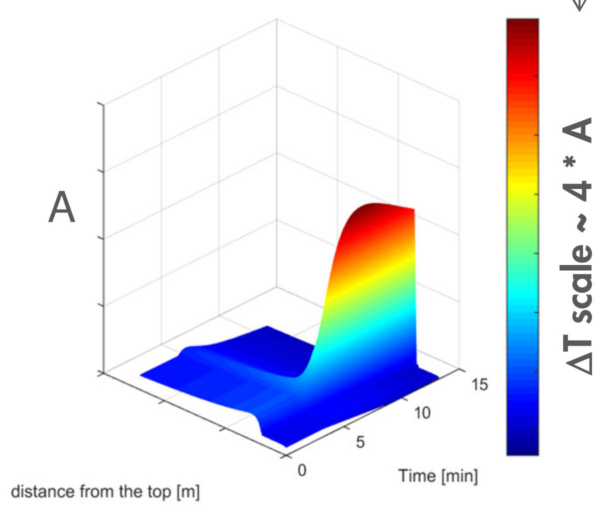
This allows us to improve operating procedures and adjust catalyst activity across the reactor to minimize impact

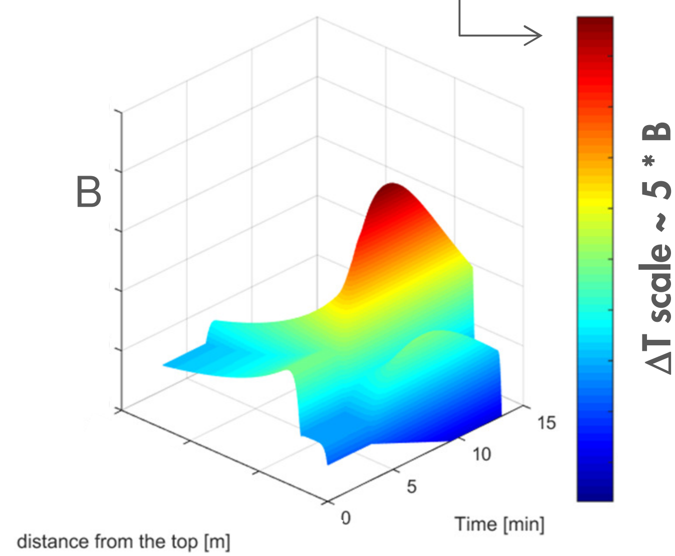
MODEL BASED OPTIMIZATION OF RESPONSE TO UPSETS

Non – optimized case: significant excursion; with high likelihood of catalyst degradation

Optimized case: minor temperature increase with hardly any catalyst performance implications

Scales are different: A = 4B



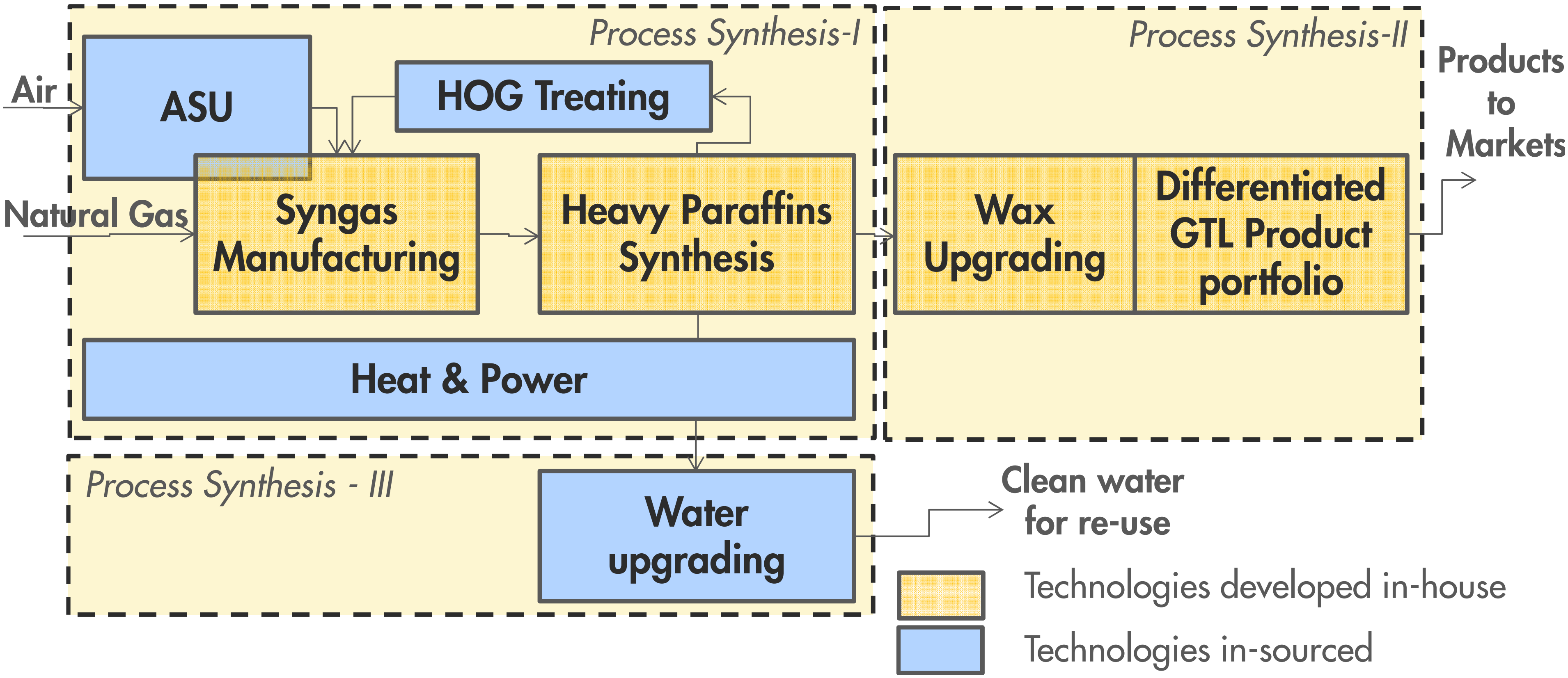


- Pilot plant tests are expensive and time consuming
- Dynamic simulations help to understand reasons, conditions & implications of temperature excursions
- ….and allow for optimization of catalyst shape, size and activity, as well as operating conditions → quick screening of options

4.2

Process Synthesis

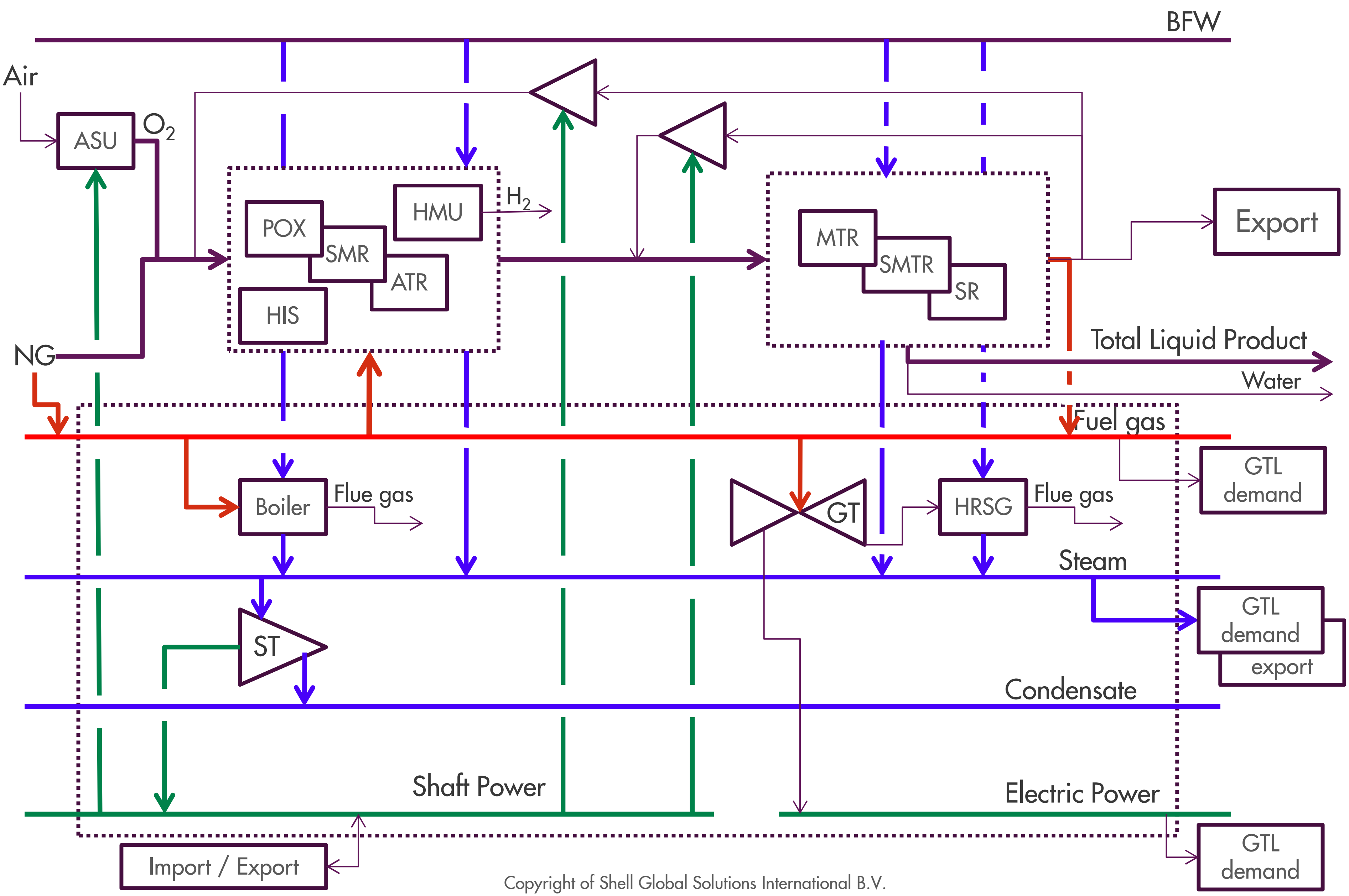
DECOMPOSITION GTL FLOWSHEET



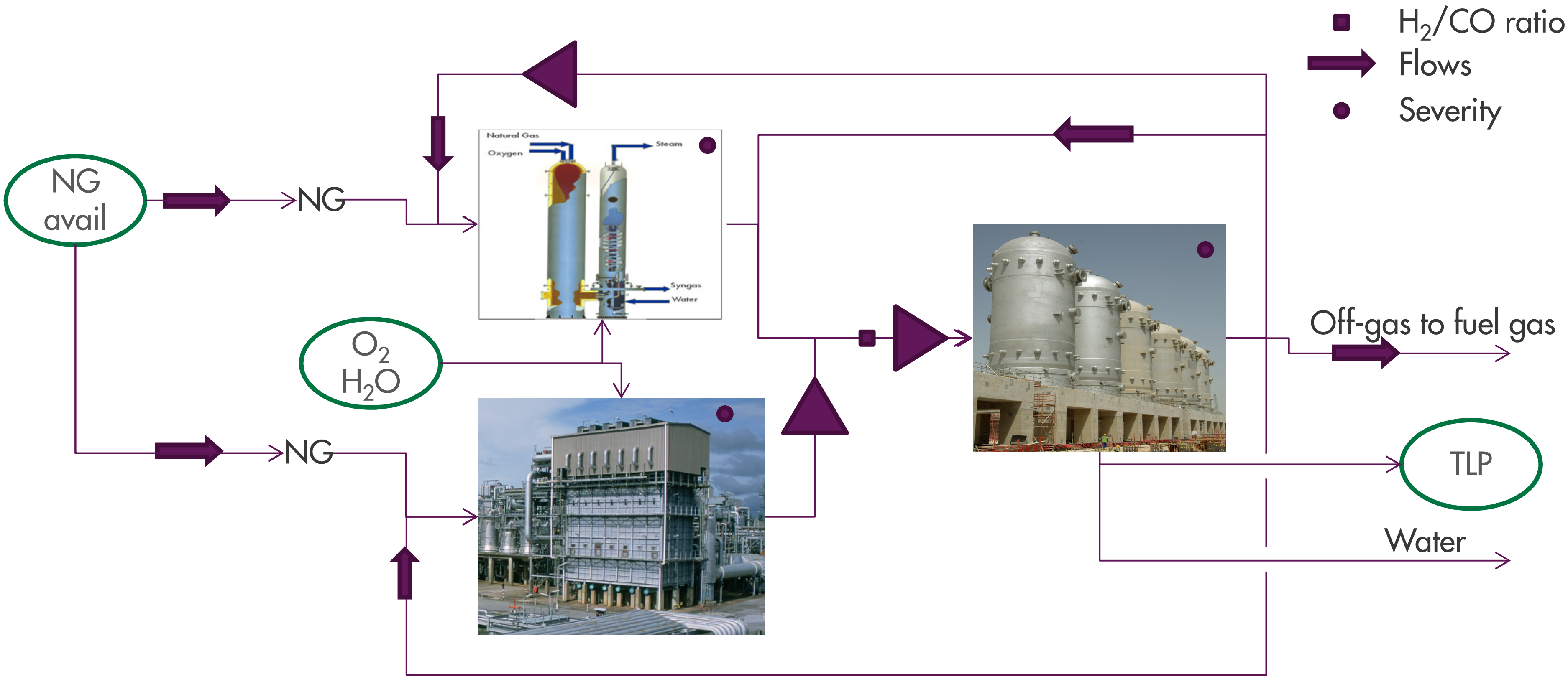
Advanced Process Modelling approaches for these Process Synthesis challenges

- ***I → GTL Process Synthesis Tool → MINLP***
- ***II → Marginal Profitability → MILP***
- ***III → MINLP / Heuristics approach***

SCOPE PROCESS SYNTHESIS TOOL

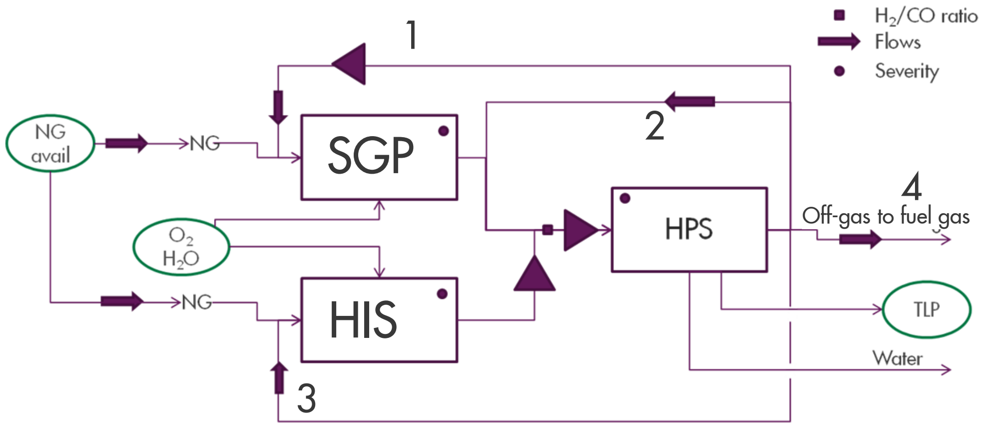


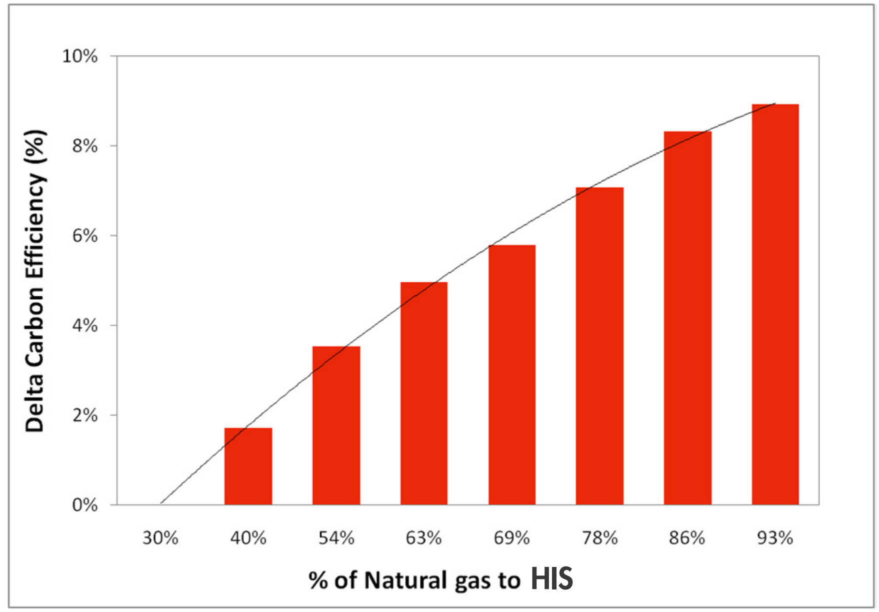
CASE STUDY: OPTIMIZATION SYNGAS PRODUCTION

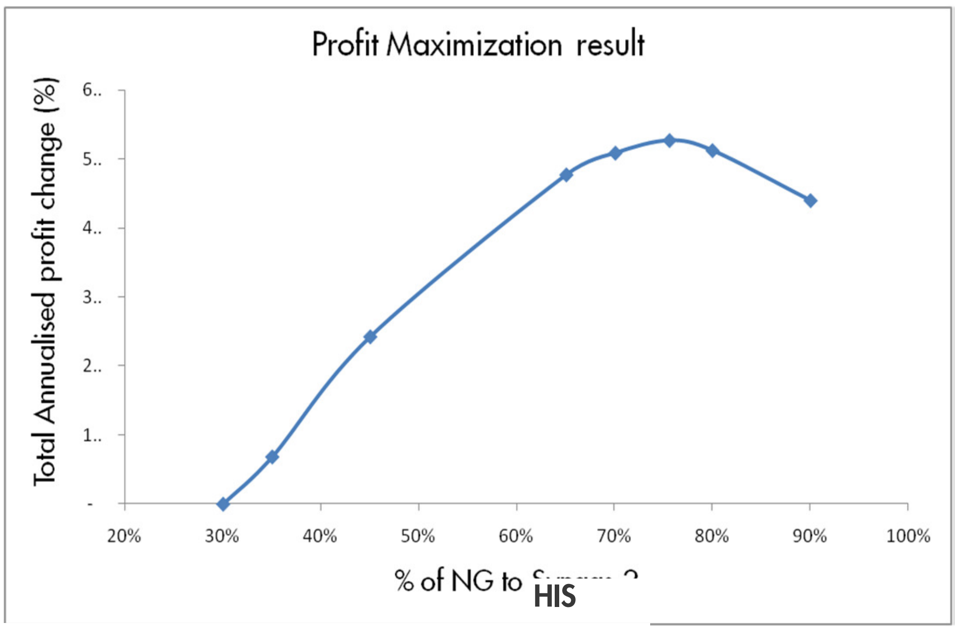


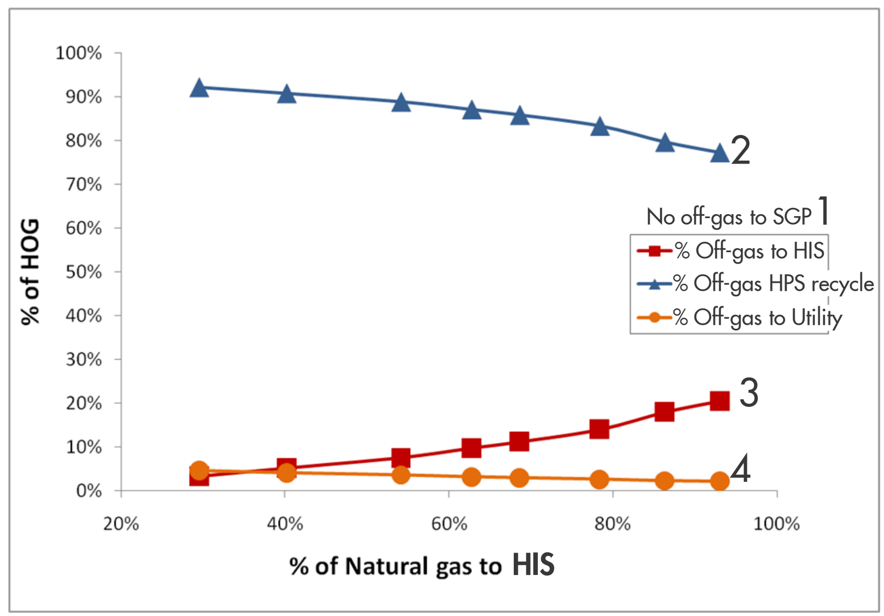
- HIS is more efficient than SGP, but is also more expensive
- How to balance syngas make: carbon efficiency vs. economic value
- 10 on/off choices → 1024 process evaluations

CASE STUDY RESULTS









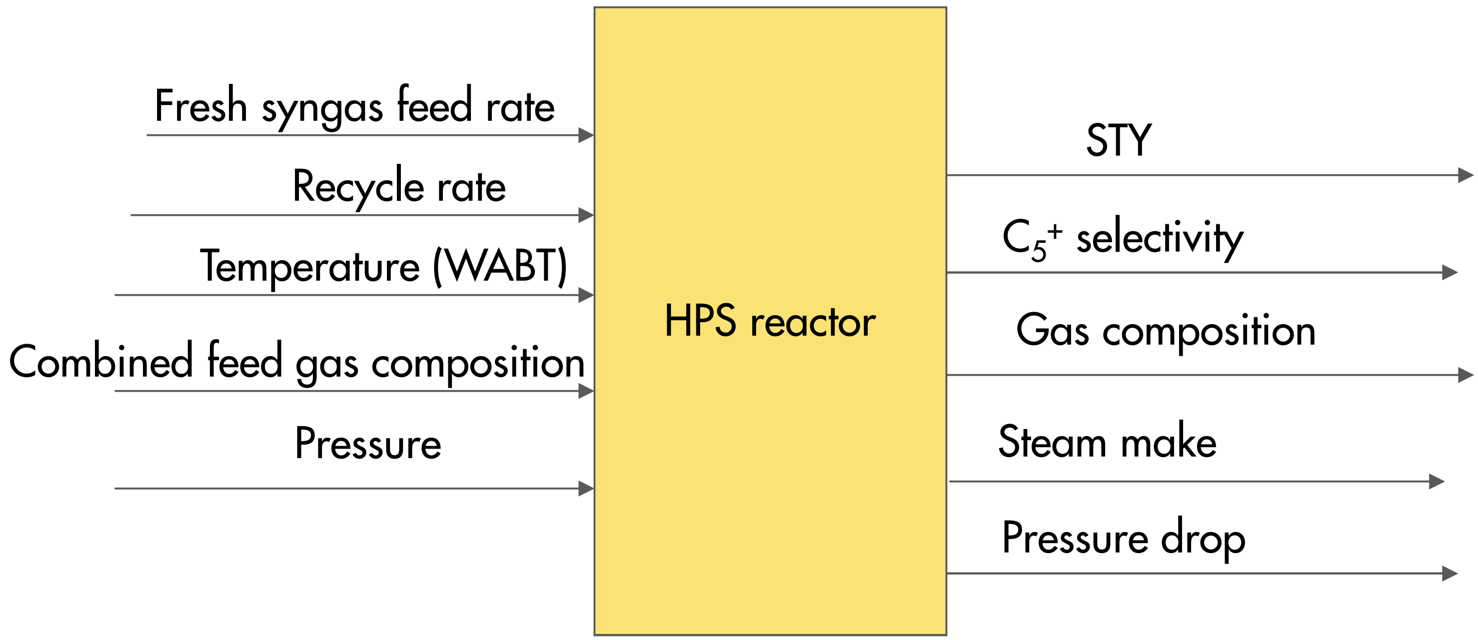
4.3

Optimisation & APC

DAY-TO-DAY OPTIMIZATION HPS REACTOR SECTION

- An integrated model for the HPS section has been developed within AIMMS to optimize the performance of individual HPS reactors, starting from daily plant data.
- Given are the amounts of fresh syngas available with its composition from various sources, catalyst activity per reactor, separator operating conditions and # of HPS reactors available
- The objective is to maximize HPS wax yield
- Degrees of freedom per reactor: feed flow, inlet composition, temperature, pressure.
- Constraints per reactor: max allowable pressure drop, temperature operating window, outlet composition requirements;
- Constraints for the entire section: off-gas surplus to be send to fuel gas system

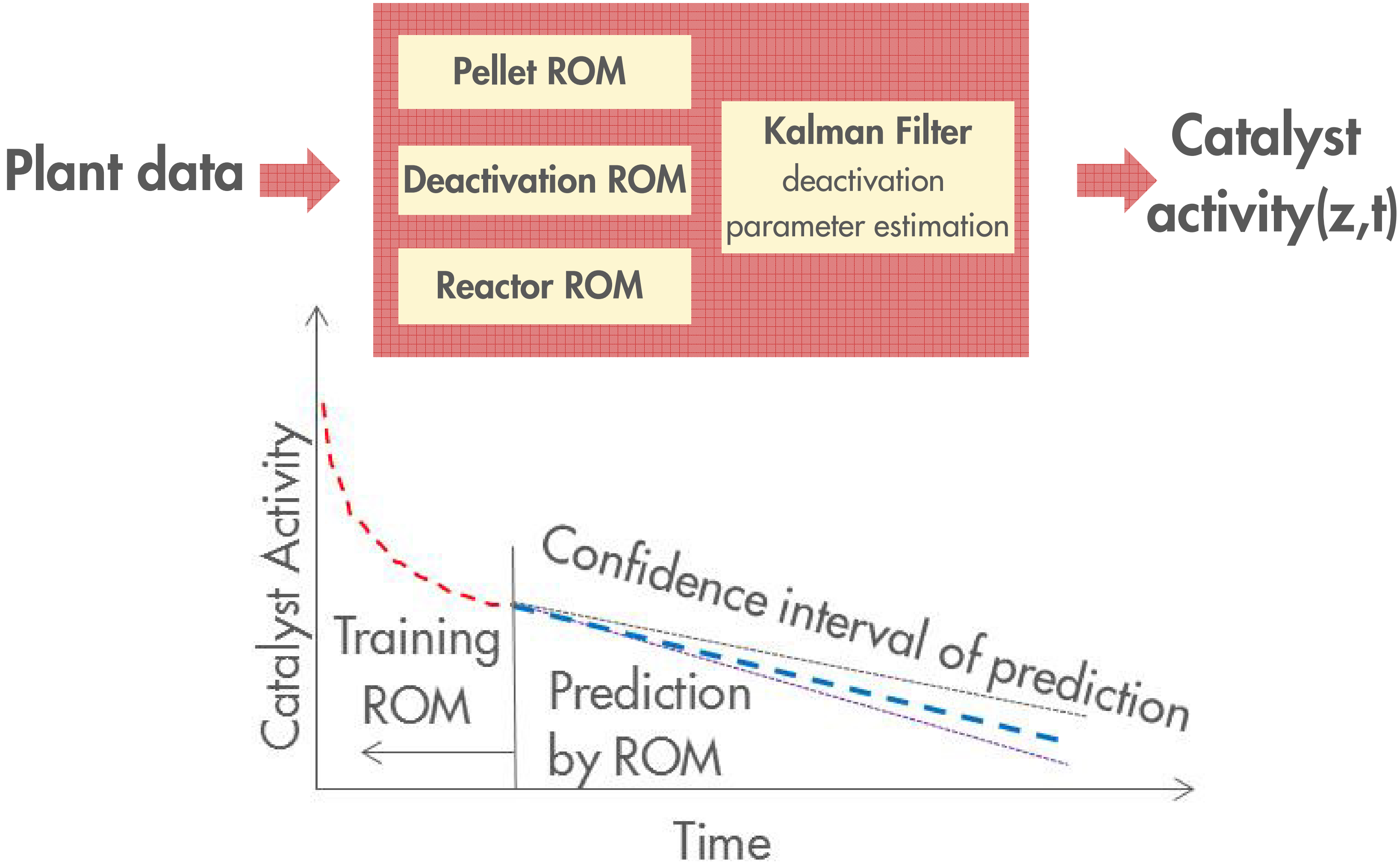
DYNAMIC SIMULATIONS SUPPORT DESIGN OF MODEL PREDICTIVE PROCESS CONTROL FOR HPS REACTORS



- An HPS reactor is a complex unit with multiple inputs & outputs.
- Once optimal performance targets are set, Model Predictive Control (MPC) is deployed to maintain these targets
- gPROMS based dynamic simulations help to design MPC's

4.4 Catalyst Deactivation

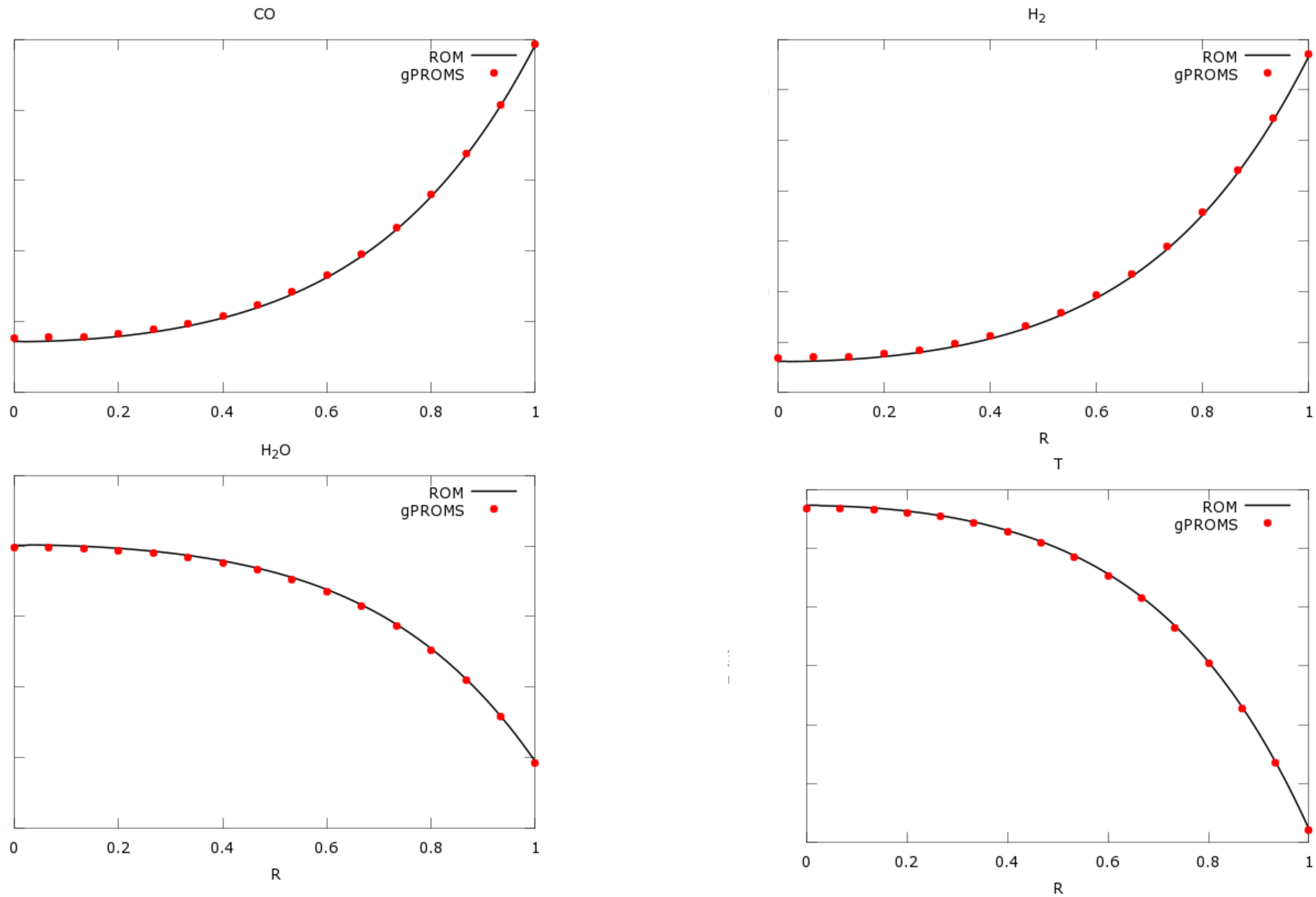
PROJECTING DEACTIVATION: GREY-BOX APPROACH



→ ***More reliable estimation of catalyst deactivation with time***

→ ***Basis for Dynamic Optimisation (future work)***

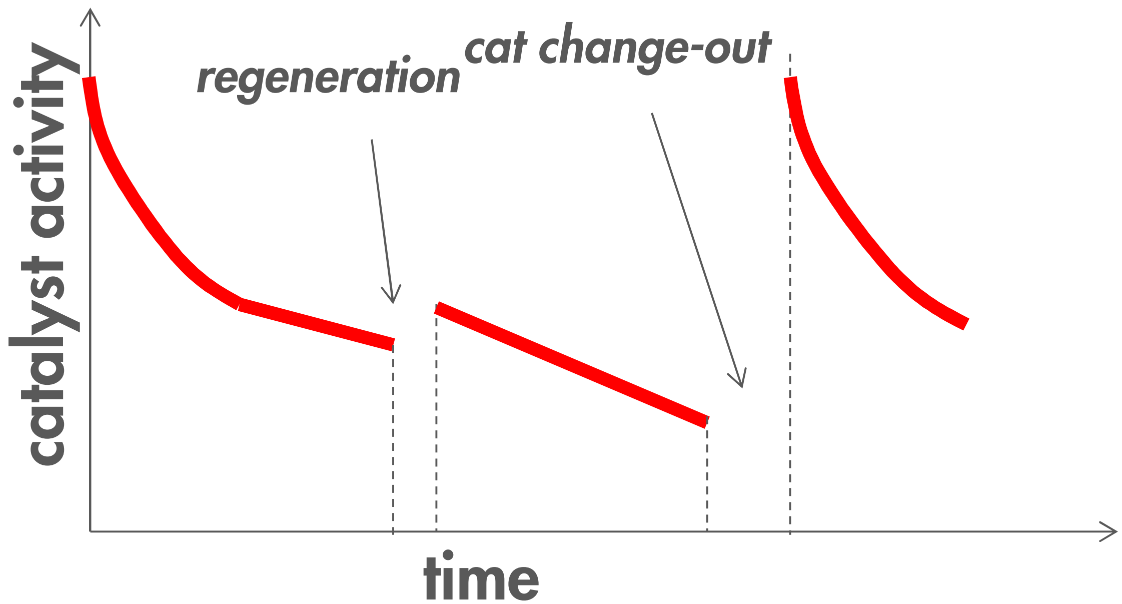
CATALYST PELLET PROFILES: REDUCED ORDER MODEL VS gPROMS



→ ***Excellent agreement of ROM with high fidelity gPROMS model***

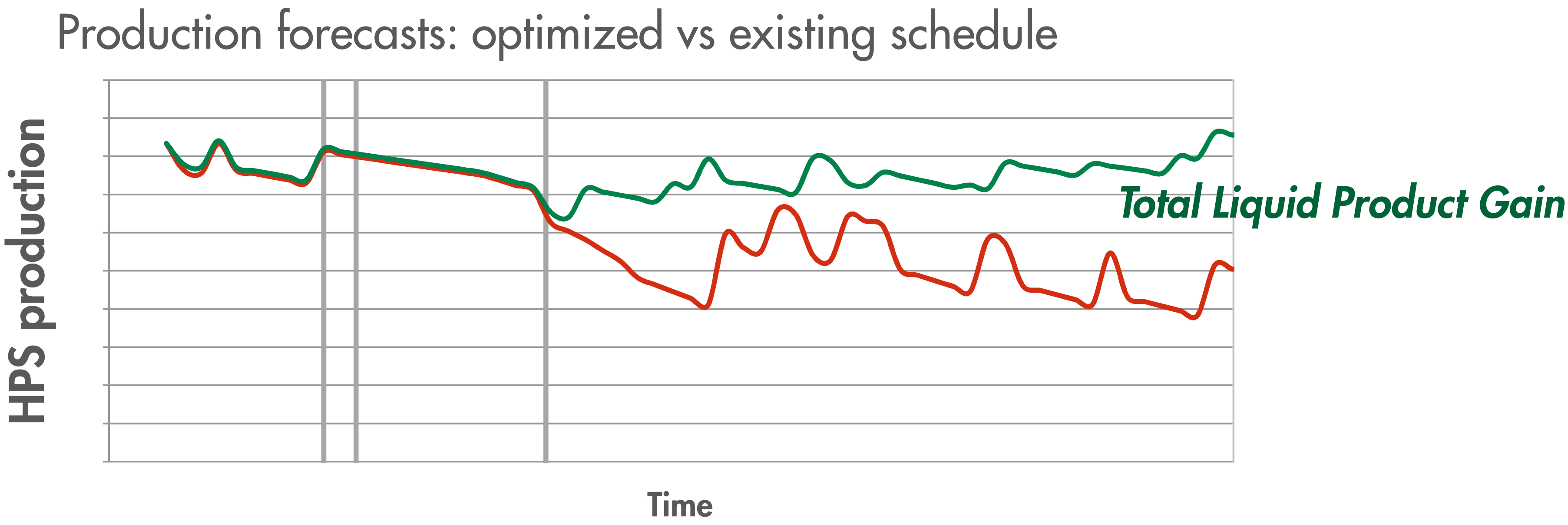
4.5
Catalyst Change Out optimization

CATALYST REGENERATION & CHANGE OUT OPTIMIZATION



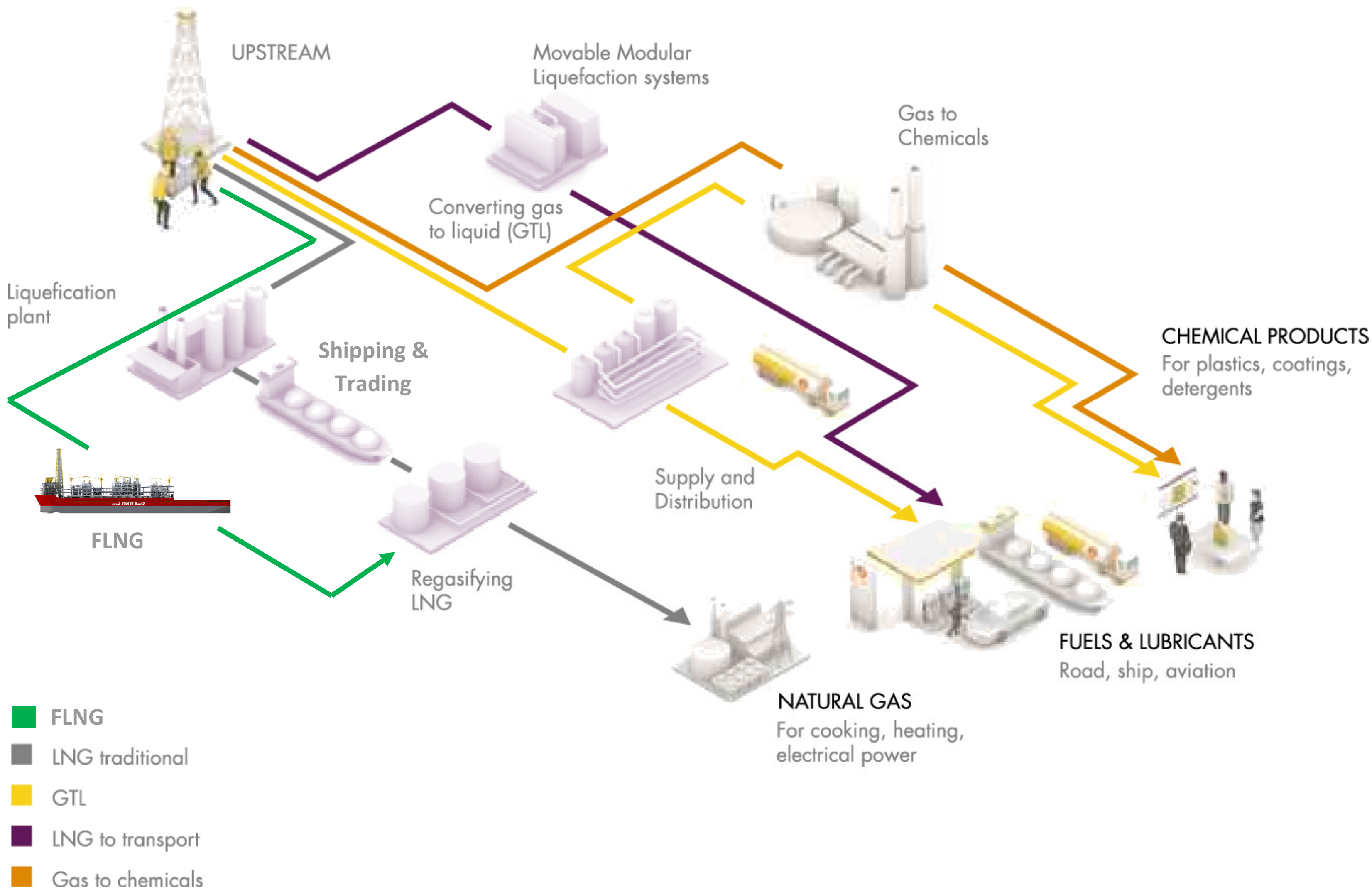
- To maintain wax production over time, catalysts have to be regenerated or replaced by a new batch
- Challenge is to find schedule of regenerations / change-outs such that over time wax revenues from corrected for regen and C/O costs are maximized while also considering availability of cat regeneration / activation unit
- This gives a mixed integer non-linear problem with a very large number of decision variables (24 reactors times 2-4 years time horizon -> 10000 variables)
- Simulated annealing as robust optimization approach in support of a reliable advise to Pearl GTL
- → AIMMS based Cat Scheduler tool in support of catalyst change-out planning & business planning as well as new projects scoping

CASE STUDY: REGENERATION & CHANGE OUT OPTIMIZATION

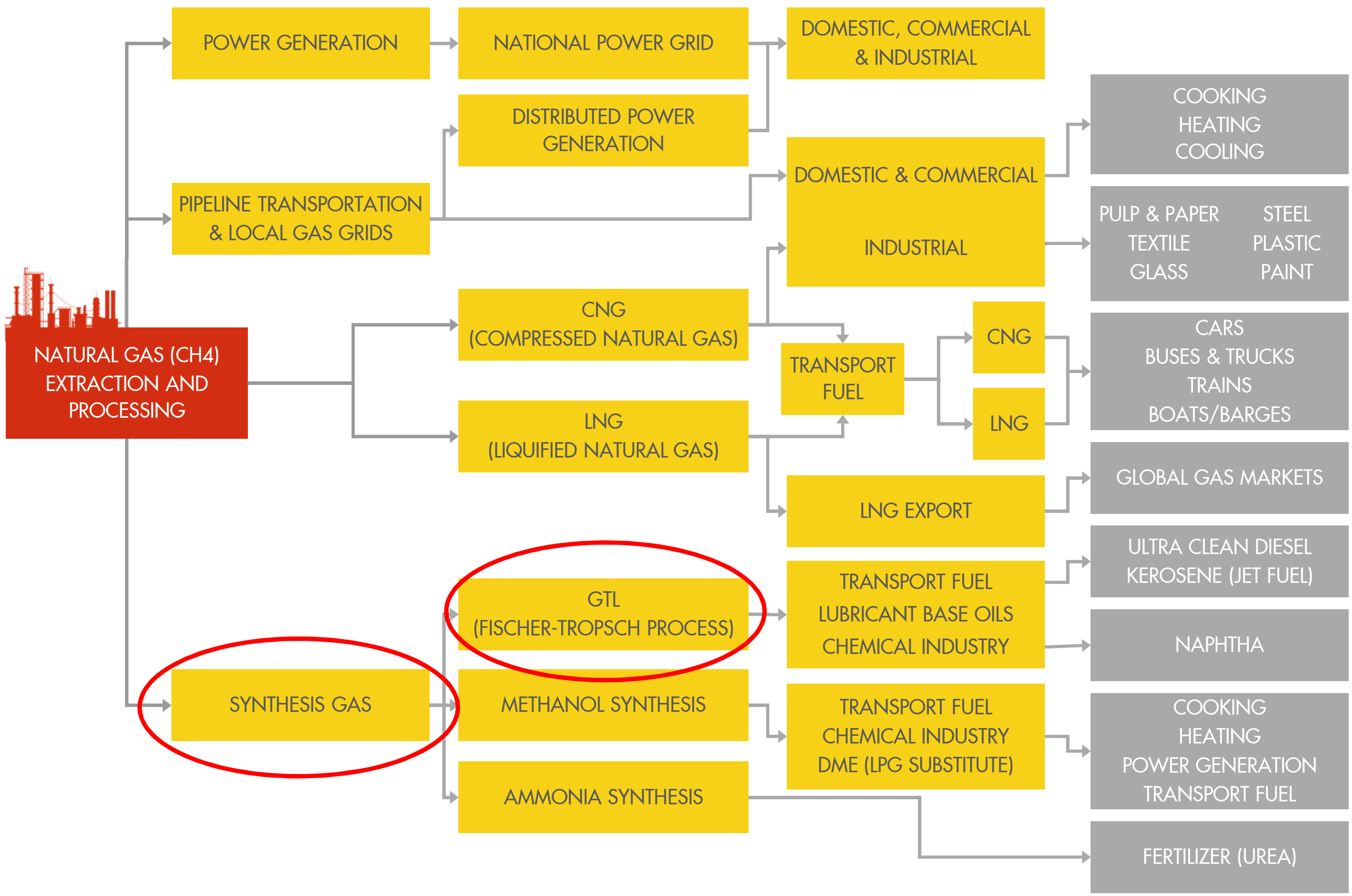


4.6
Gas Value Chain Studies

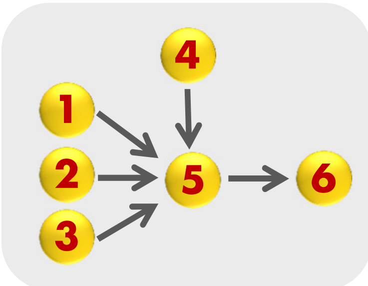
COMPETITIVENESS GTL AGAINST ALTERNATIVES



GAS MONETISATION OPTIONS



APPROACH TOWARDS GAS VALUE CHAIN STUDIES



Strategic Input
- Aspired portfolio of products
- Supply & Demand scenarios
- Outlook on Prices & Costs

4

Value Chain Analysis
- Economic Valuation
- Investment over time analysis

5

6

Credible, Affordable, and Competitive Value Chain Options

Supply
- Gas availability, quality & cost
- Availability of water, power
- Prices of gas, water, power
- Supply logistics and costs

1

Conversion Infrastructure
- Yields,
- Capital data
- Variable & Fixed Costs

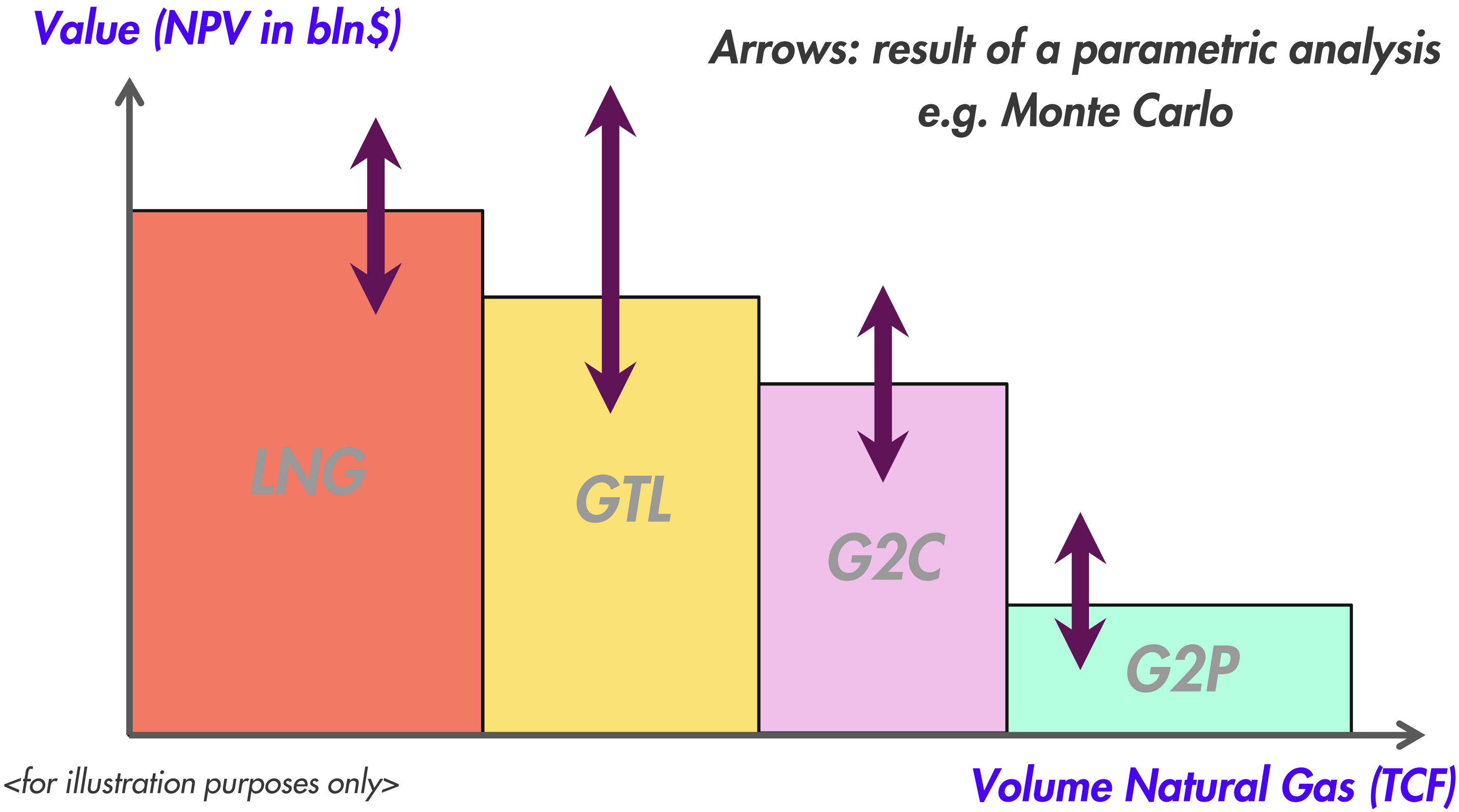
2

Demand
- Definition of demand areas
- Product demand & price data
- Distribution network
- Transportation options & costs

3

Parametric analysis (e.g. Monte Carlo) gives targets for GTL Technology Development → GTL remains the Value Proposition of choice for Major Resource Holders over time

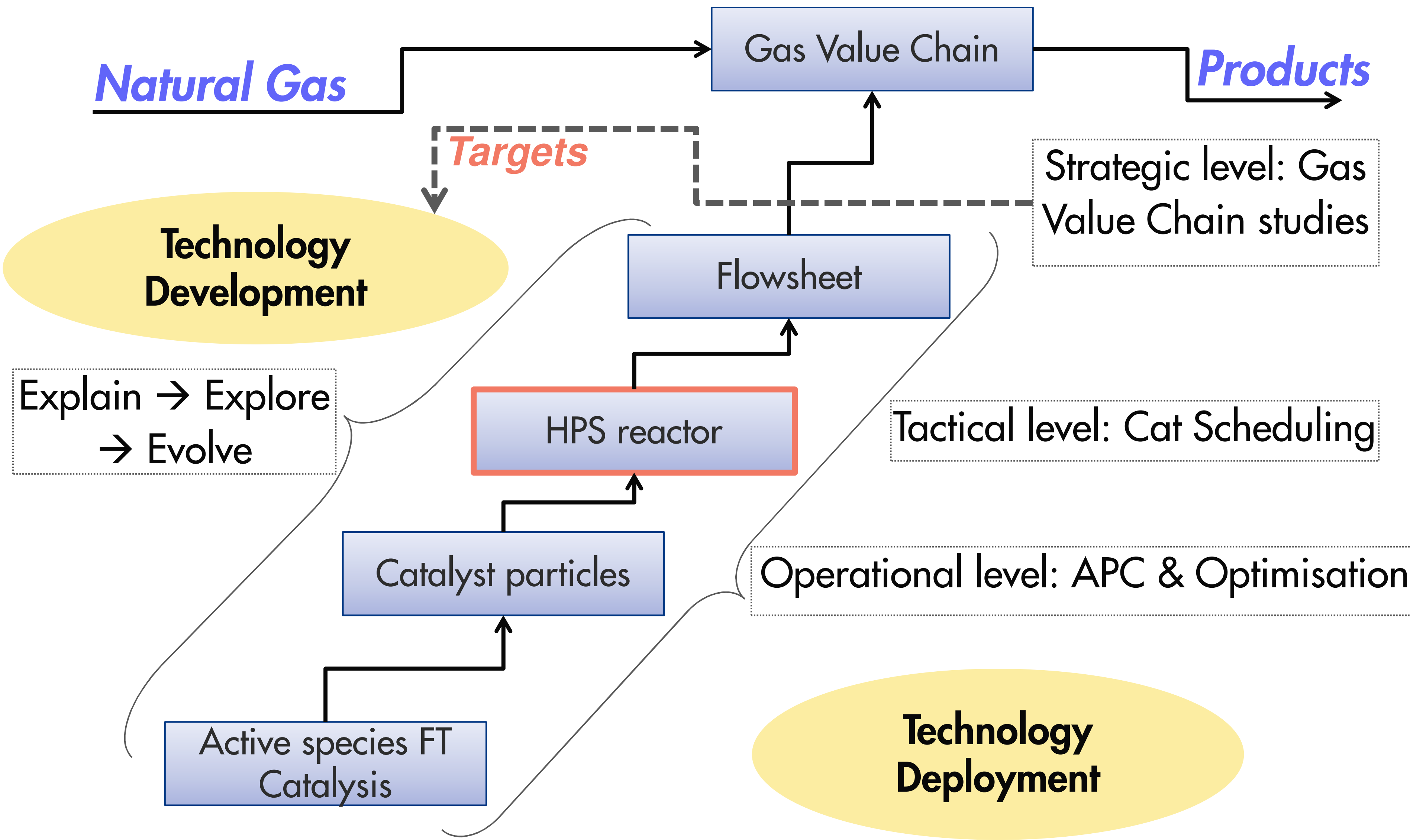
RELATIVE ATTRACTIVENESS STUDY OUTCOME: NETBACK TO MAJOR RESOURCE HOLDER



5

Summary & Conclusion

ADVANCED PROCESS MODELLING ENABLES VALUE CREATION



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