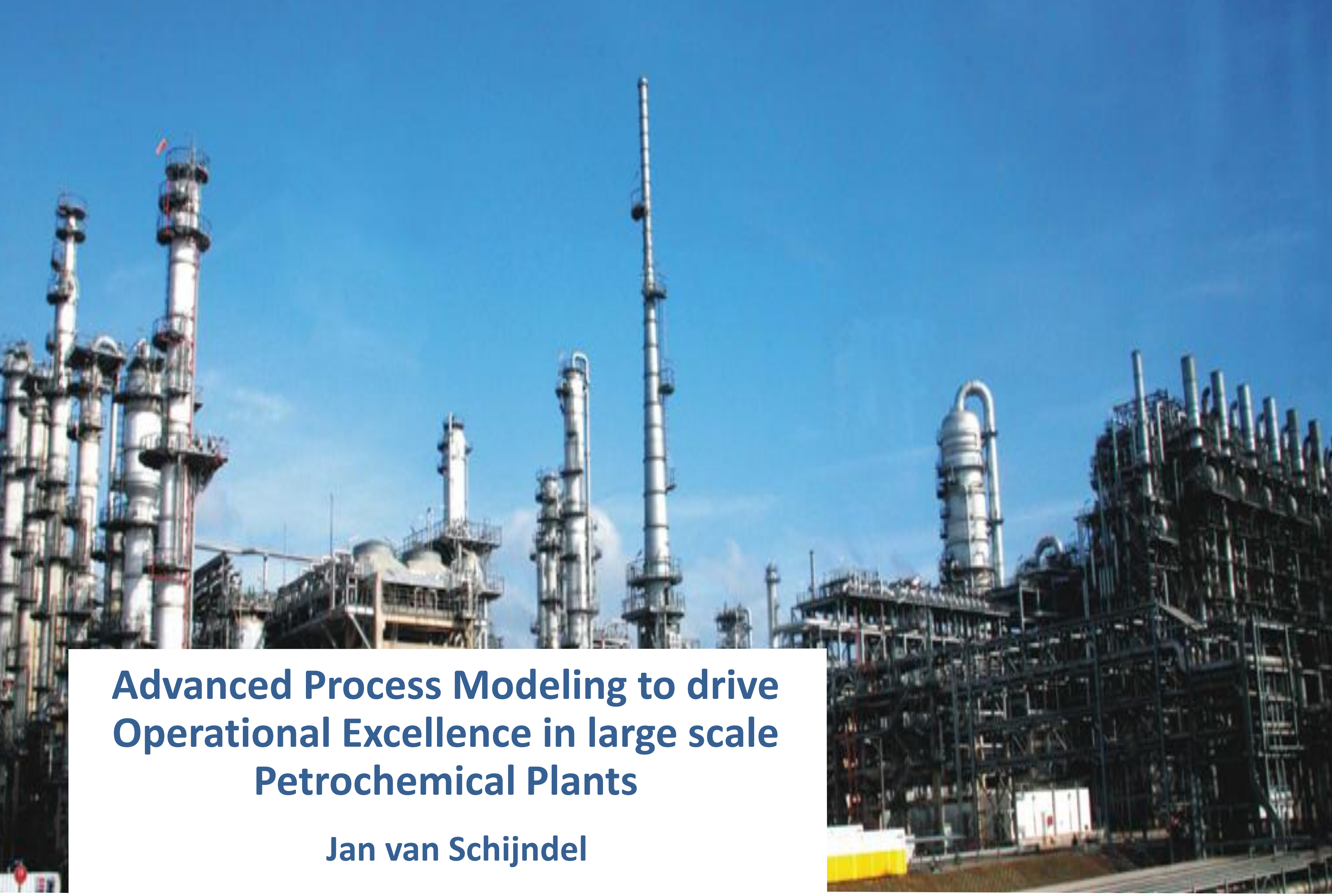


Advanced Process Modeling to drive Operational Excellence in large scale Petrochemical Plants

Jan van Schijndel

Outline

- **Advanced Process Modeling**
- **Challenges for Petrochemical Producers**
- **Operational Excellence for Olefins Production**
- **Olefins Optimization Framework**
- **Summary & Outlook**

ADVANCED PROCESS MODELING

ADVANCED PROCESS MODELING

Definition

- Advanced Process Modeling concerns the development of High-Fidelity predictive process models within an Equation-Oriented modelling & Optimisation platform

Advantages

- One single platform for process design → online monitoring & optimisation → multi-period production planning
- Model can be tuned to predict operational performance for accuracy needed → the "high-fidelity" element
- Combines Optimisation & Dynamic Simulation functionalities
- Lower cost of ownership

KEY FEATURES

Equation-oriented power

- Solves large-scale optimisation problems – including multiple or complex recycles – rapidly & robustly, using parallelisation to speed up solution where needed.

Multiple applications with same high-fidelity predictive model

- Steady-state & dynamic simulation / optimisation
- Parameter estimation
- Data reconciliation & State estimation
- Global system analysis
- Multi-site, multi-period optimisation

CHALLENGES PETROCHEMICAL PRODUCERS

CHALLENGES PETROCHEMICAL PRODUCERS

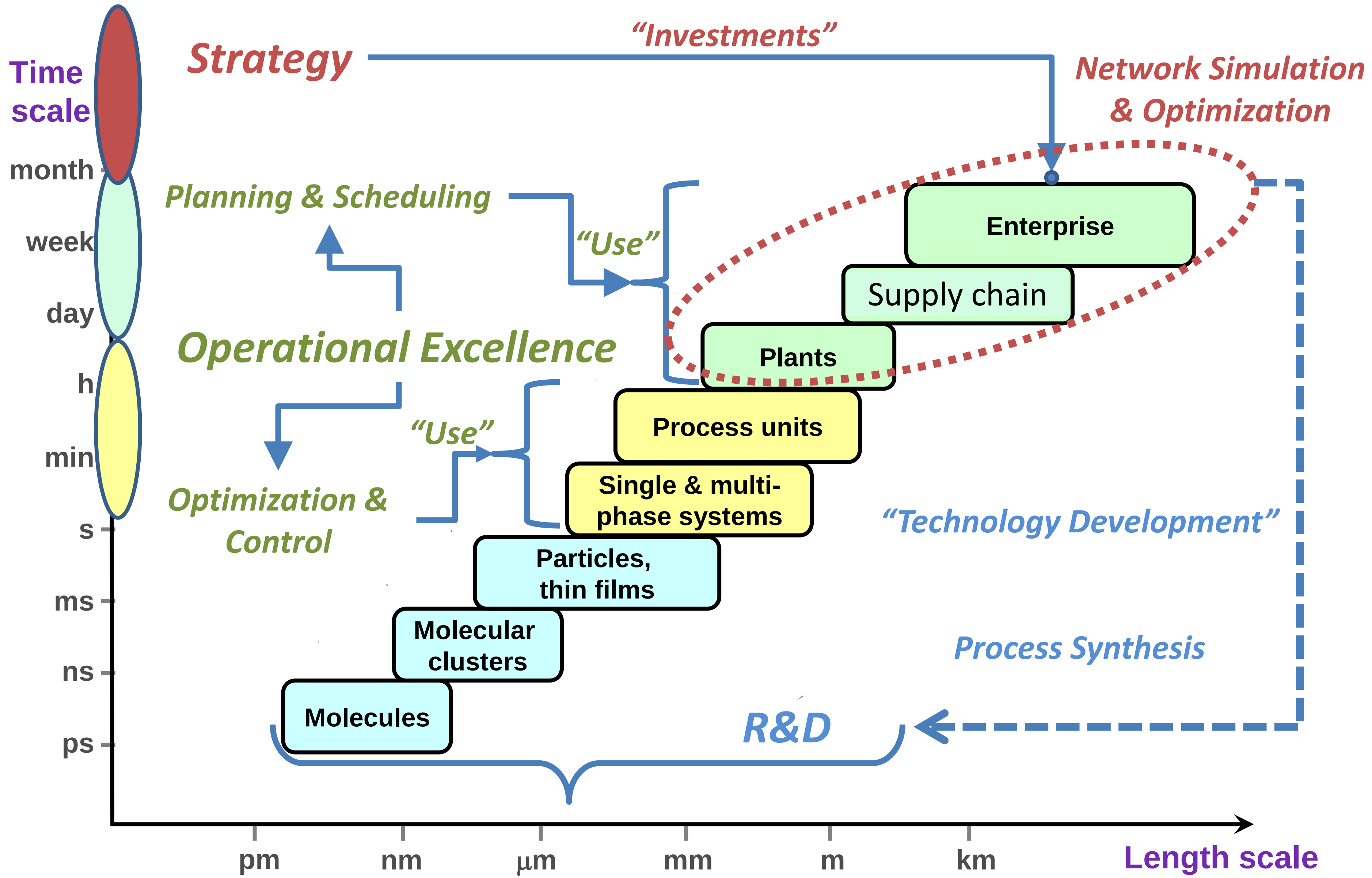
- Business Continuity

- Which investments for which markets & products? ***Strategy***

- Which technologies to develop? ***R&D***

- How to make best use of the assets? ***Operational Excellence***

ADVANCED PROCESS MODELING DECISION FRAMEWORK



OPERATIONAL EXCELLENCE FOR OLEFINS PRODUCTION

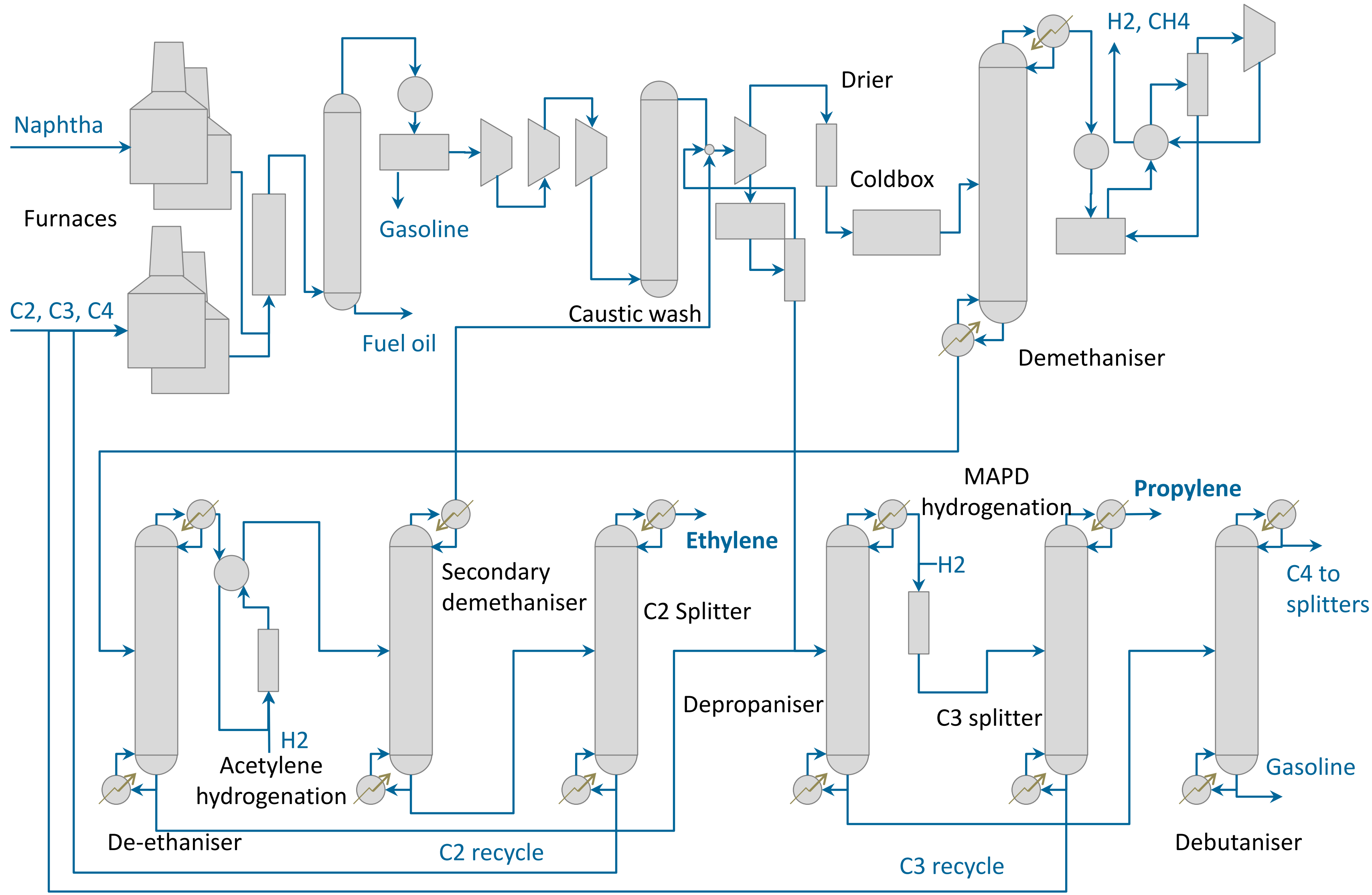
OLEFINS MANUFACTURING TECHNOLOGY

I. Pyrolysis of paraffins:
   - Decomposition of hydrocarbons by adding heat (to drive endothermic reactions)
   - Hydrogen abstraction and recombination reactions yield lower olefins & heavy hydrocarbons (aromatics & naphthalenes).
   - Steam is added to influence residence time (τ) and partial pressure of hydrocarbons (P_{hc})
   - Yields are a function of residence time (τ) , temperature (T) and pressure (P) over the cracking coil

II. Compression & Deep Cooling to get almost all components liquefied

III. Fractionation into "pure" product streams by gradual release of pressure & simultaneously warming up

SIMPLIFIED FLOW-SCHEME OLEFINS PLANT



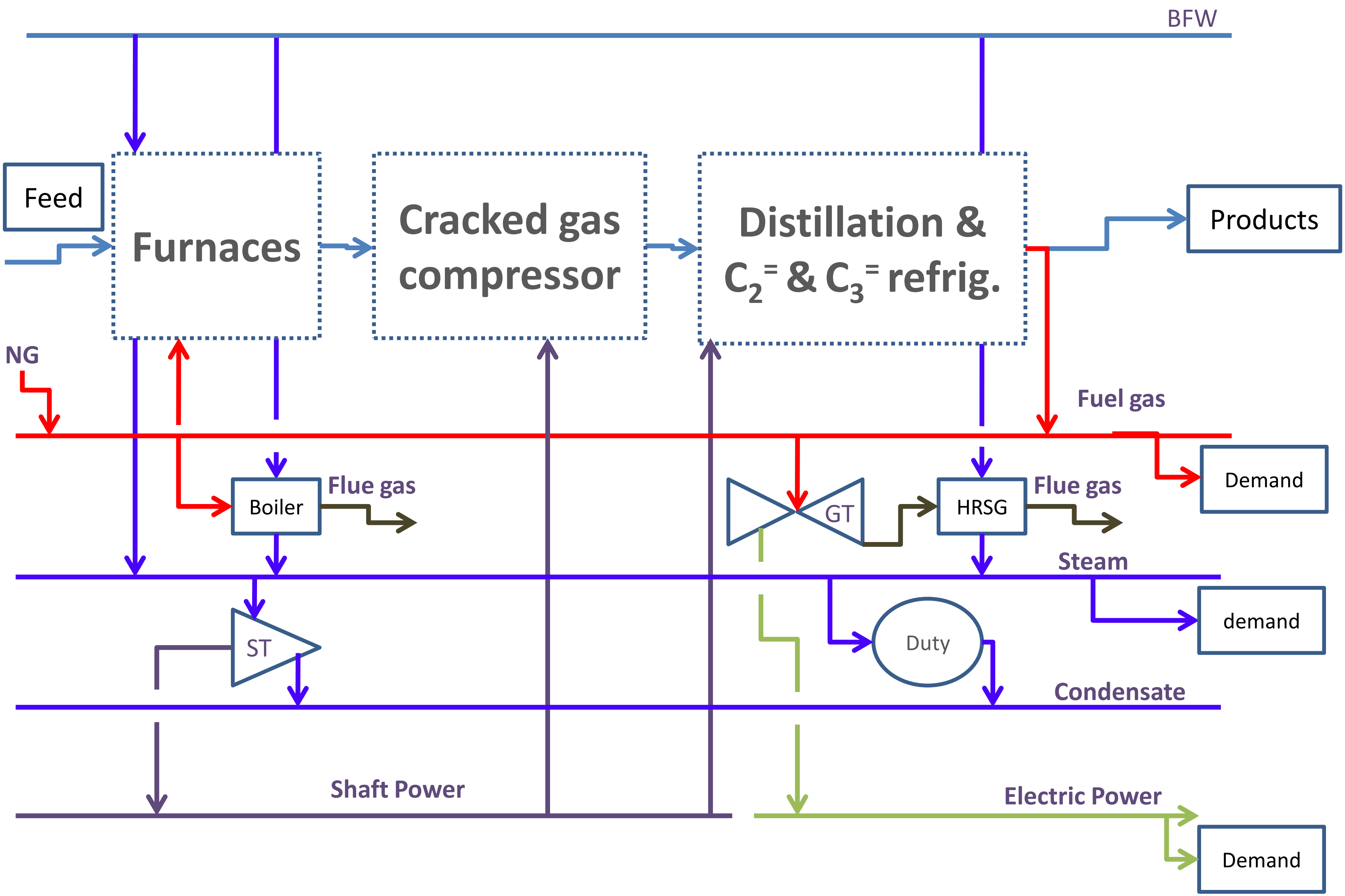
FURNACE SECTION OLEFINS PLANT

Typical furnace capacity: 100 t/h feed @ 25% yield on ethylene per pass

@ 6 + 1 philosophy

→ 1.25 mln ton $C_2^=$ per year

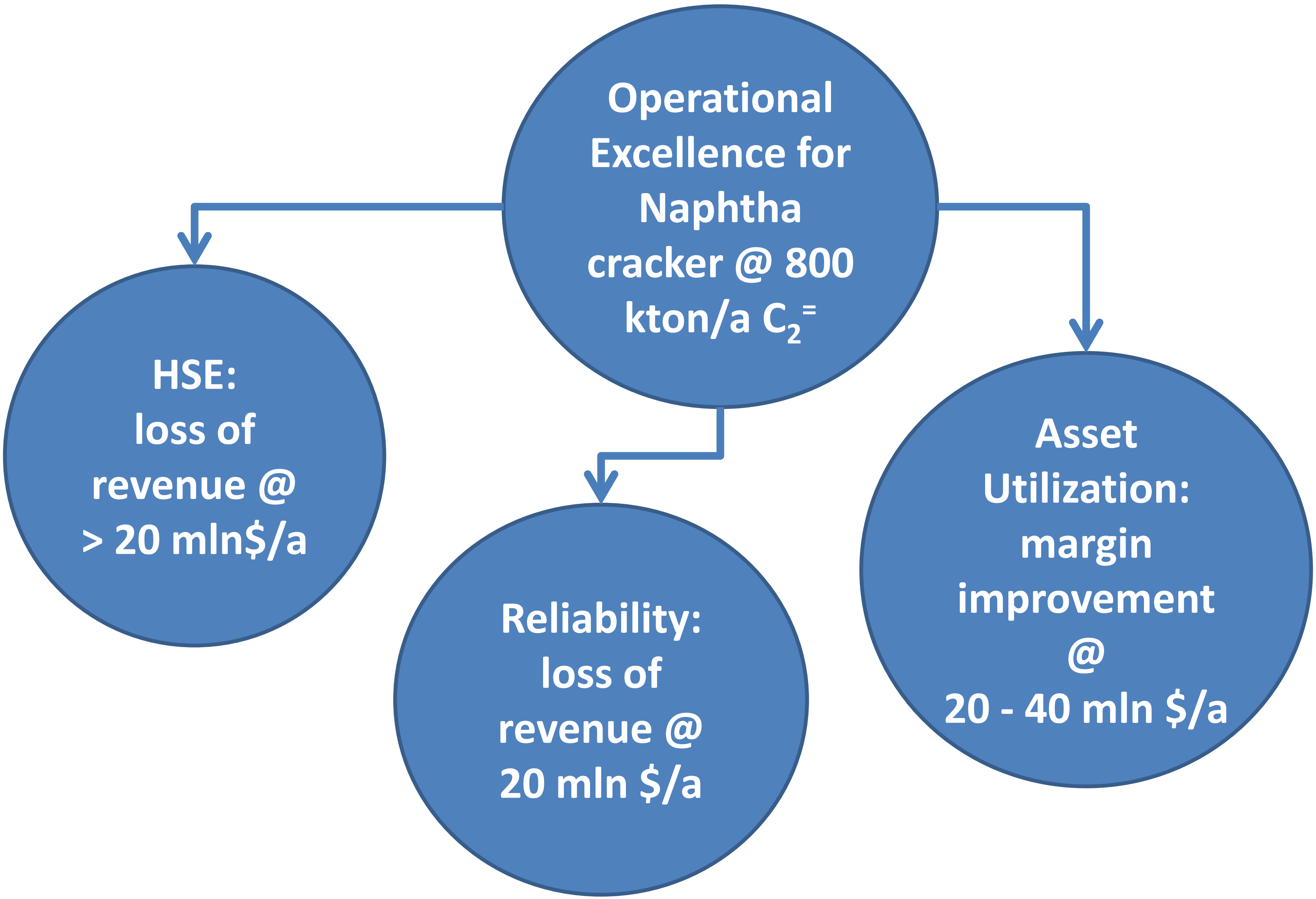
HEAT & POWER BALANCE OLEFINS PLANT



OLEFINS MANUFACTURING ECONOMICS

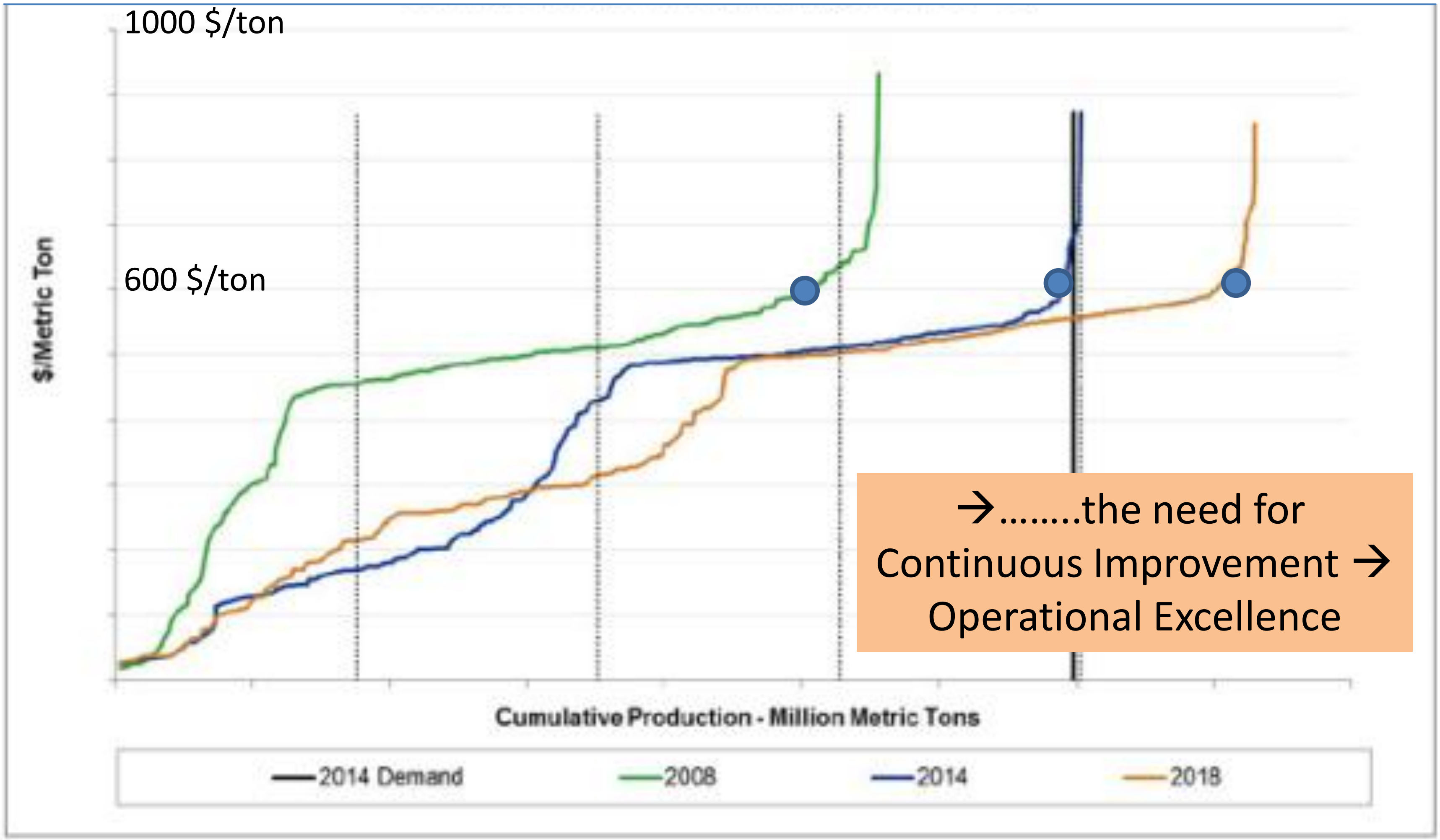
- Capacity: 800 kton of ethylene per year
- Investment: 2 bln\$ @ 2500 \$/ton $C_2^=$
- Cash costs: 600 \$/ton $C_2^=$ based on:
  - Nett Hydrocarbon Feedstock Costs: 310 \$/ton $C_2^=$
    @ 30% ultimate $C_2^=$ yield; 80 \$/bbl Brent; uplift ~150 \$/ton byproduct
  - Specific Energy Consumption: 190 \$/t $C_2^=$
    20 GJ/ton $C_2^=$ @ 10 \$/MMBTU
  - Fixed costs: 100 \$/t $C_2^=$
    4% of investment
- Cash margin: 400 \$/ton $C_2^=$ (@ 1000 \$/ton $C_2^=$)
- Value over Investment Ratio: 0.25 (pay-back time < 6 years)

"VALUE" OPERATIONAL EXCELLENCE



ETHYLENE COST SUPPLY CURVE

Benchmarking
Solomon Associates - IHS



HOW TO IMPROVE SUPPLY COST POSITION?

- Radical:
  - Developing alternative processes with Q_1/Q_2 economics: e.g. MTO
  - New build @ larger capacities → economies of scale; higher efficiency
  - **Debottlenecking** → lower unit fixed costs (~ 10 $/ton $C_2^=$) & better energy efficiency (5% lower SEC → 10 $/ton $C_2^=$); assume same yield pattern
  - Debottlenecking economics: assume base load 800 ktpa increased to 1000 ktpa @ 1500 $/ton $C_2^=$ → investment 300 mln $; cash cost reduction of 20 $/ton → cash margin of 420 $/t → Improvement: 1000 ktpa * 420 $/t – 800 * 400 $/t = 100 mln $/a → VIR ~ 1.6 (pay-back < 3 years)

- Evolutionary:
  - Continuous improvement of asset utilisation → **Operational Excellence**:
    - Buy more favorable feedstock package @ 2 $/bbl → 20 $/ton $C_2^=$
    - Operate for a more attractive yield pattern @ 2% better uplift → 7 $/ton $C_2^=$
    - Operate @ 3% lower energy consumption → 6 $/ton
    - Total 33 $/ton lower cash costs → 26 mln $/a
  - Key enabler: **Advanced Process Modeling & Optimization**

OLEFINS OPTIMIZATION FRAMEWORK

UTILIZATION CHALLENGES OLEFINS PRODUCERS

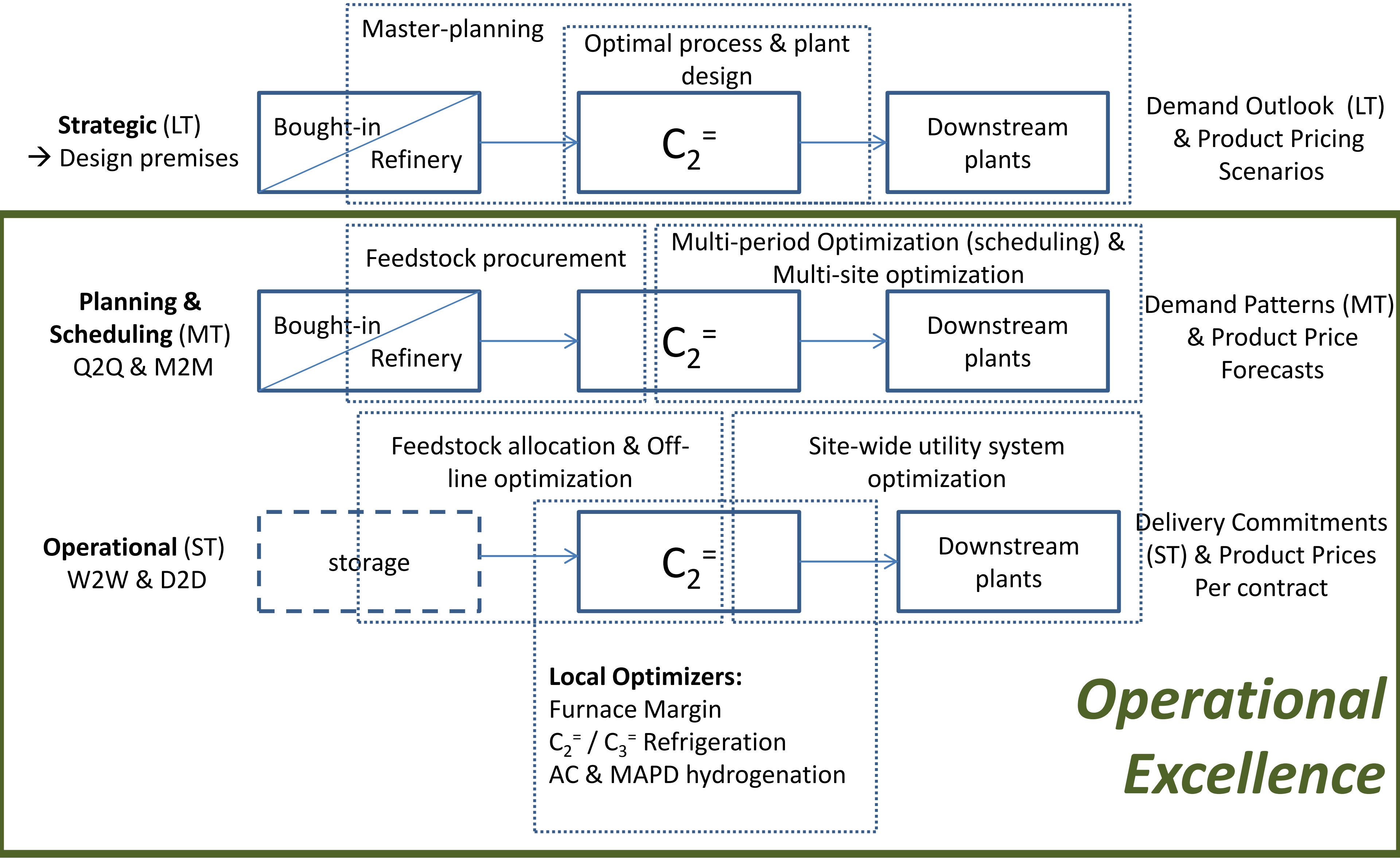
- Buy feeds with highest upgrading potential, for a given downstream product portfolio: *feedstock procurement challenge*

- Process feeds such that margin potential is captured at lowest possible energy consumption within major plant limitations: *furnace allocation challenge*

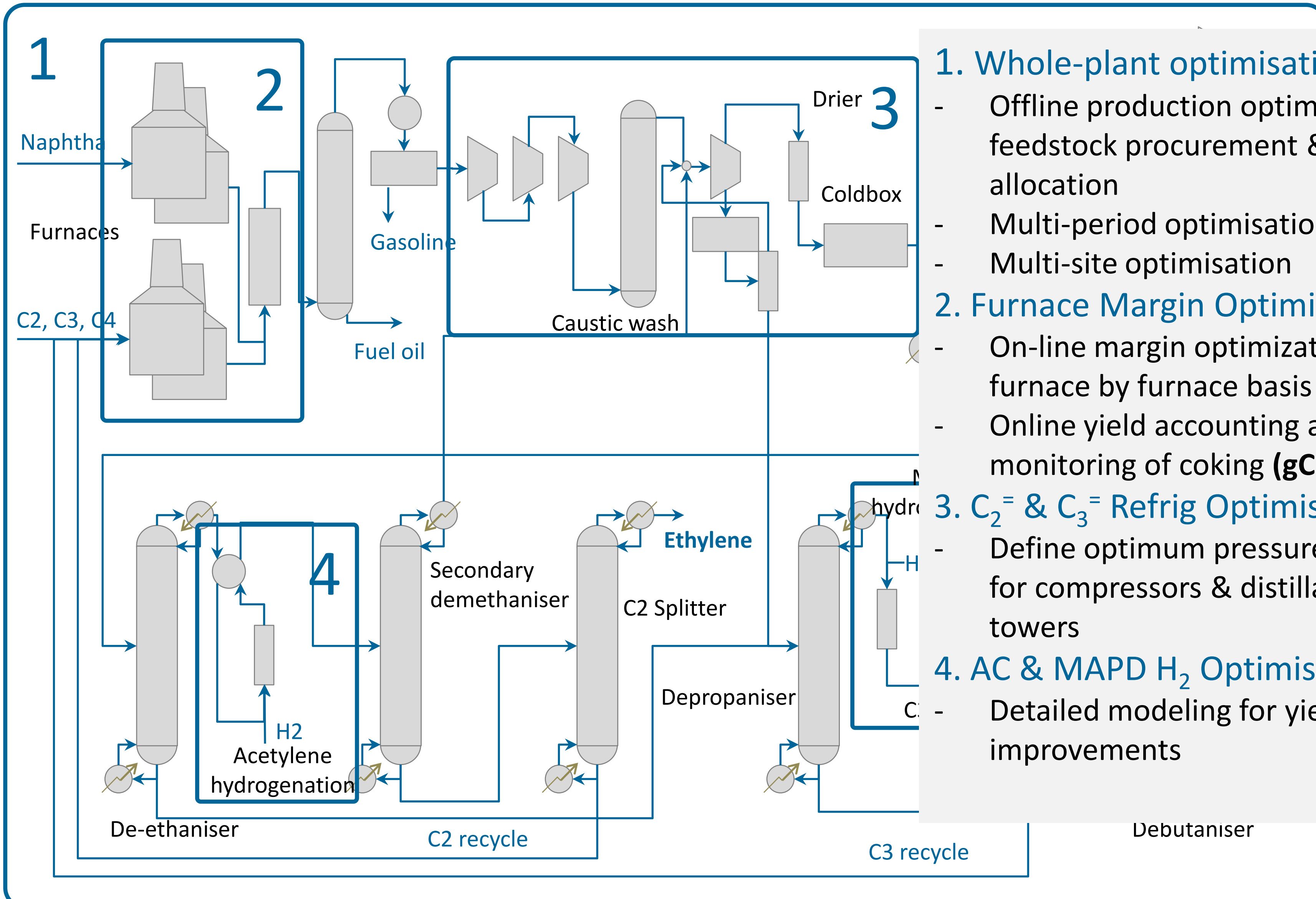
- "Sweat the assets": *Local Optimization & Advanced Process Control challenge*

- Adjust operating conditions when needed to exploit market opportunities and/or manufacturing & logistic constraints; both upstream; in-plant; and downstream: *off-line optimization challenge*

OLEFINS DECISION SUPPORT FRAMEWORK



OPERATIONAL EXCELLENCE OLEFINS PLANTS: WHERE OPTIMISATION ADDS VALUE



1. Whole-plant optimisation

- Offline production optimisation: feedstock procurement & furnace allocation
- Multi-period optimisation
- Multi-site optimisation

2. Furnace Margin Optimisation

- On-line margin optimization on a furnace by furnace basis
- Online yield accounting and monitoring of coking **(gCRACKER)**

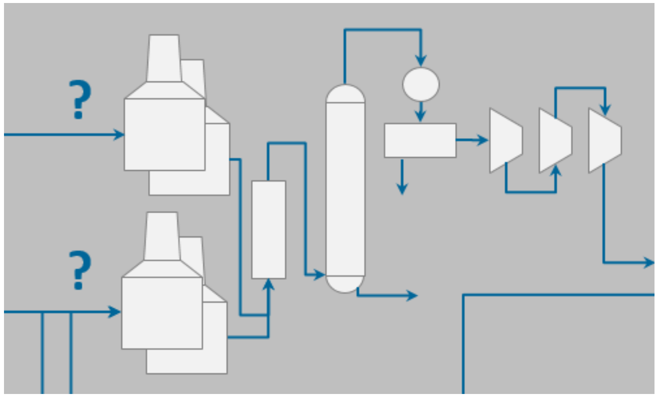
3. $C_2^=$ & $C_3^=$ Refrig Optimisation

- Define optimum pressure levels for compressors & distillation towers

4. AC & MAPD H_2 Optimisation

- Detailed modeling for yield improvements

FEEDSTOCK ALLOCATION



Background:

- Many plants have a mix of different furnace types & capacities & the option of processing different feedstocks.
- Product requirements change from week to week

Scope: whole plant model

Operational Challenge:

- Decide which feeds to run through which furnaces and at what conditions (feed rate, severity, STOR) also given the state of coking in each furnace
- Consider impact on the back-end of the plant e.g. operation of the downstream separation system with constraints imposed by refrigeration system capacity. Also the rate of C_2, C_3 and perhaps C_4 recycles need to be taken into account (which in turn affects feedstock allocation)

Benefit: a higher revenue stream

- Better asset utilisation due to higher furnace throughputs
- Lower energy consumption and hence a lower CO_2 footprint
- More valuable product mix

FURNACE MARGIN OPTIMIZER

Detailed furnace model estimates:

- Cracking Yields
- Coke build-up over run length
- Heat recovery

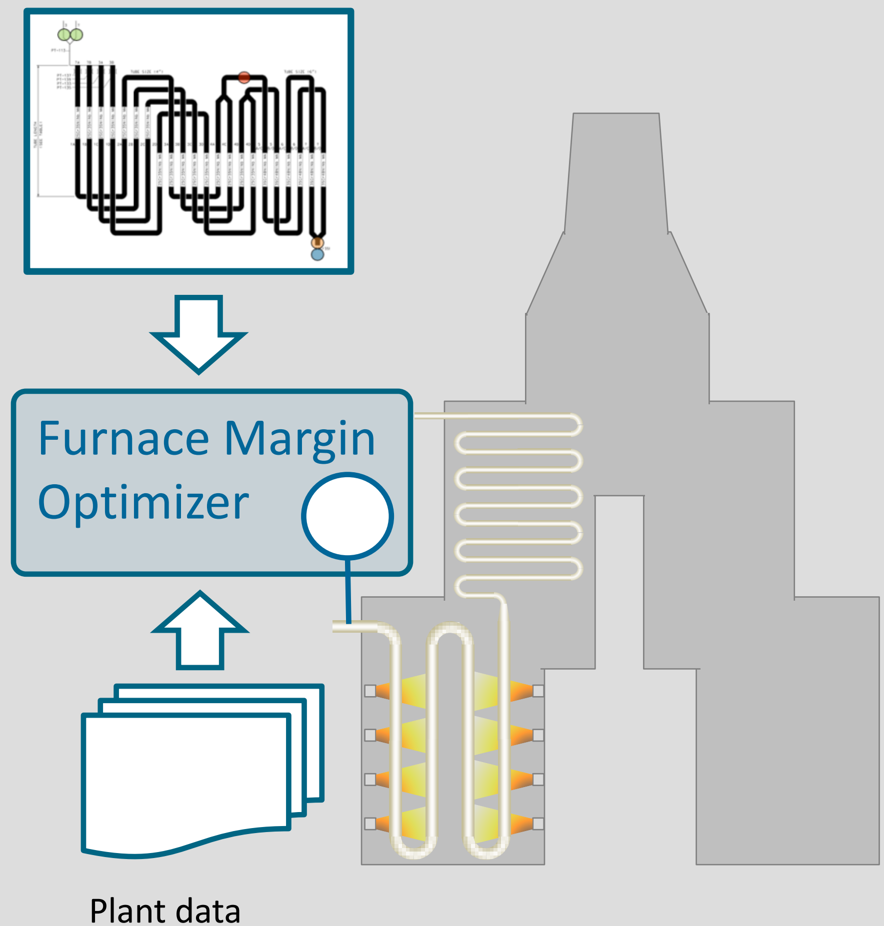
Combines:

- Cracking & coking kinetics for any coil geometry, fired duty, heat recovery convection section & TLE
- State estimation technology to reconcile performance estimates with available furnace data (feed rate, effluent composition, CIT, COT)

Benefits:

- On-line margin optimization on a furnace by furnace basis
- Better furnace utilization through advanced EOR projection for decoke scheduling
- Solid basis for dynamic optimization entire furnace section

Scope Furnace Model: Coil + Convection Section + Radiant Box + TLE



ACETYLENE & MAPD HYDROGENATION

Scope:

- Fixed bed reactor models for conversion of Acetylene (C_2H_2) & Methyl Acetylene and PropaDiene to Ethylene (C_2H_4) and Propylene (C_3H_6)

Objective function:

- Maximise acetylene / MAPD conversion for maximum ethylene & propylene gains

Subject to:

- Max allowable levels of ethane and green oil production
- Allowable activity loss over time to avoid catalyst regeneration before turn-around

Degrees of freedom:

- Temperature profile over reactor
- H_2/C_2H_2 and H_2/MAPD ratio's

Support to design and engineering:

- Reactor scale-up from laboratory to pilot to commercial scale
- Tune catalytic bed properties (length, activity, shape of particles) & cooling system design to for thermal stability so to avoid hot spots during operation

PROPYLENE & ETHYLENE REFRIGERATION SYSTEMS

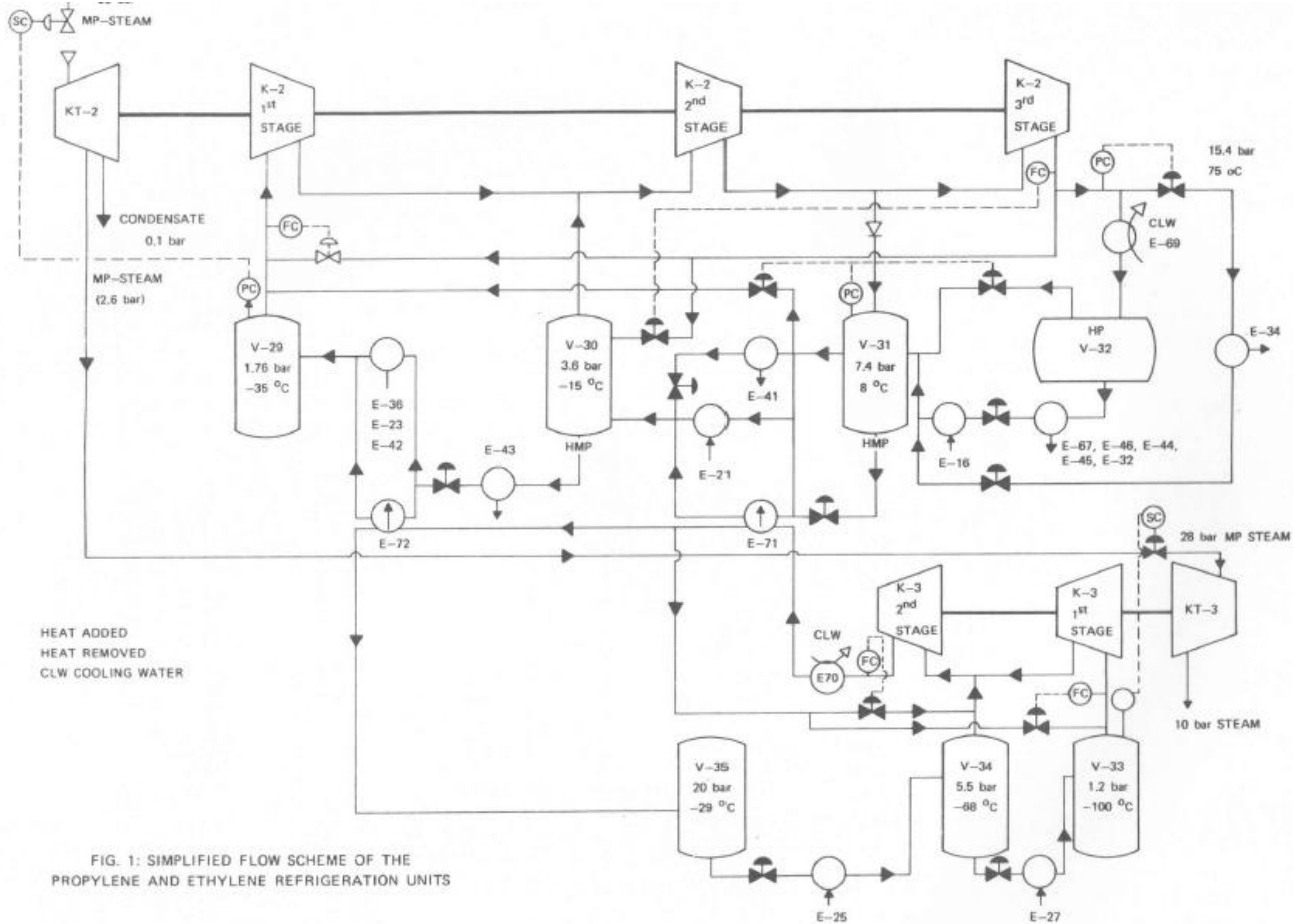
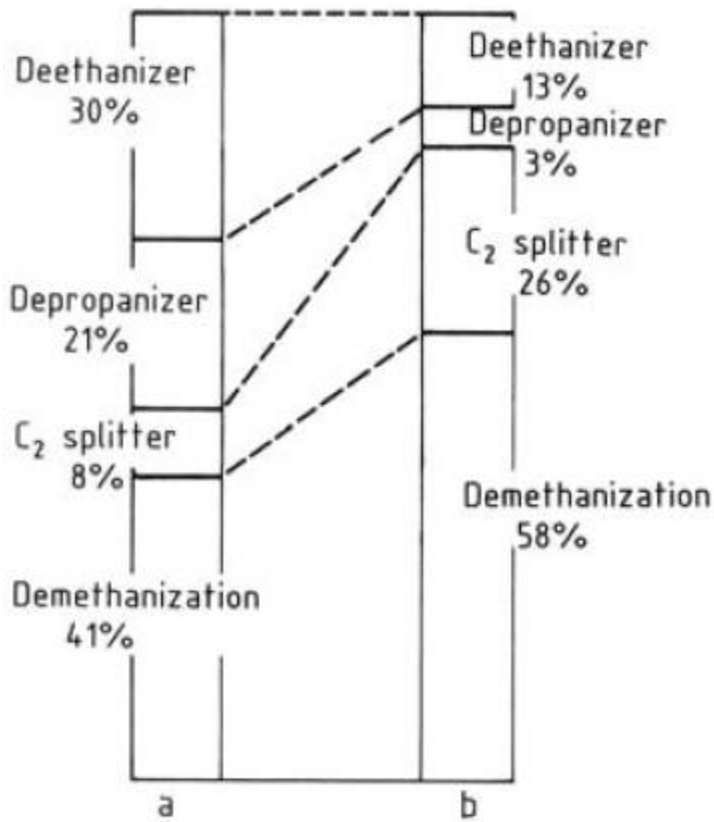


FIG. 1: SIMPLIFIED FLOW SCHEME OF THE PROPYLENE AND ETHYLENE REFRIGERATION UNITS

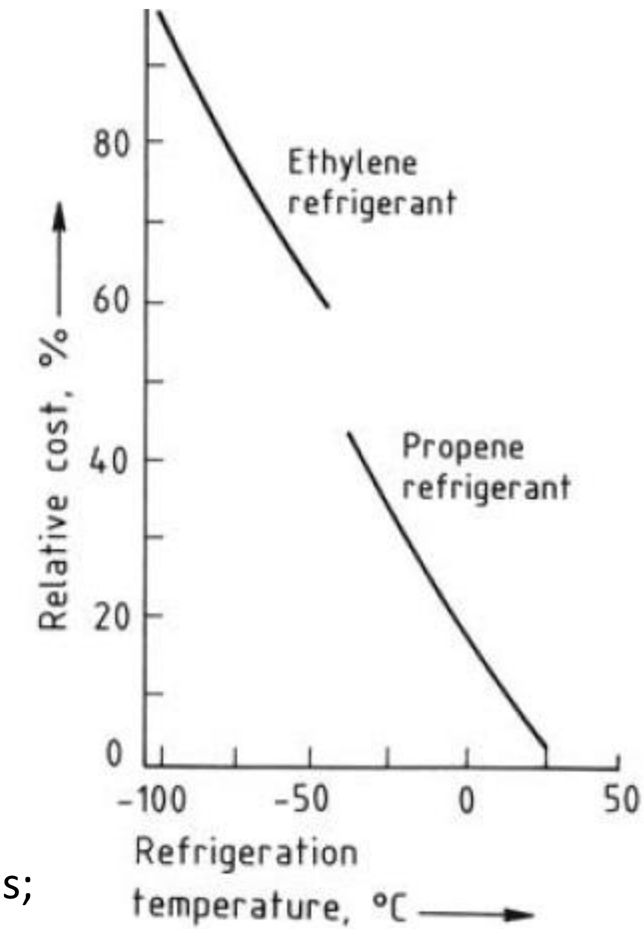
HEAT & WORK BALANCE REFRIGERATION SYSTEMS

Distribution of heat load and work requirements



a) Net heat absorbed by the refrigeration systems;
b) Net work done by the refrigeration systems

Relative cost of heat extraction by the refrigeration systems at different temperatures



OPTIMIZATION $C_2^=$ & $C_3^=$ REFRIGERATION SYSTEMS

Scope:

- $C_2^=$ & $C_3^=$ compressors, including suction, inter-stage & discharge systems
- Demethanizer feed train
- Condensors & Reboilers cold distillation columns: demethanizer, de-ethaniser, depropanizer and EE-splitter

Objective function: minimize $C_2^=$ & $C_3^=$ compression power

Subject to:

- Hydraulic limitations distillation columns
- Product quality specifications

Degrees of Freedom:

- Suction, intermediate & discharge pressures $C_2^=$ & $C_3^=$ compressors
- Tower pressures

SUMMARY & OUTLOOK

- Advanced Process Modeling supports Olefins producers addressing Operational Excellence challenges so to improve their cost of ethylene supply position:
  - Feedstock procurement; furnace allocation and capacity utilization by optimization of the furnace section within back-end limitations
  - Optimization $C_2^=$ & $C_3^=$ refrigeration cycles – AC & MAPD hydrogenation
  - Utilities optimization
  - Better integration at site and enterprise level

- Advanced Process Modeling delivers lower cash costs and a lower CO_2 footprint

- New challenges ahead for olefins (and other petrochemical) producers:
  - Increasing efforts and investments to reduce GHG emissions
  - Call for Licensors for radical process redesigns (e.g. to benefit from electrification potential) → process integration & process intensification
  - This also calls for more advanced process synthesis / optimisation approaches

- A new challenging arena for Advanced Process Modeling

Q & A