Optimization of Acetylene Hydrogenation Reactor

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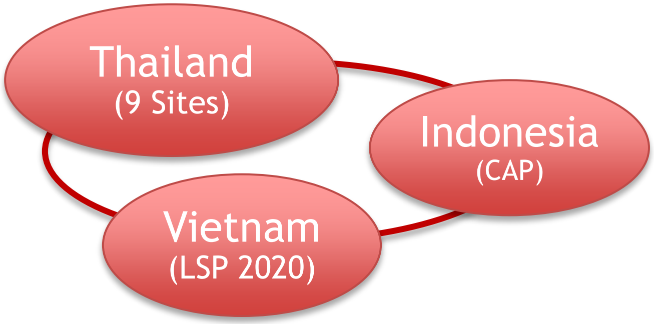
1. SCG Business Overview

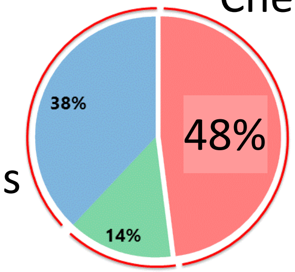
SCG Chemical is one of the largest *integrated* Petrochemical Producers in Asia

SCG Chemicals Operation



Chemicals

Cement Building Materials



Packaging

SCG Revenues FY2015

Companies : Over 200
Assets Size : US$ 14 billions
Revenues : US$ 13 billions
Employees : 60,000

Oil & Gas	Petrochemicals			Fabrication
Feedstock	**Upstream**	**Intermediate**	**Downstream** (incl. Compound/Formulation)	**Converter**

Feedstock
- Naphtha
- LPG

Upstream
- Ethylene (C2)
- Propylene(C3)
- Mixed C4
- Benzene

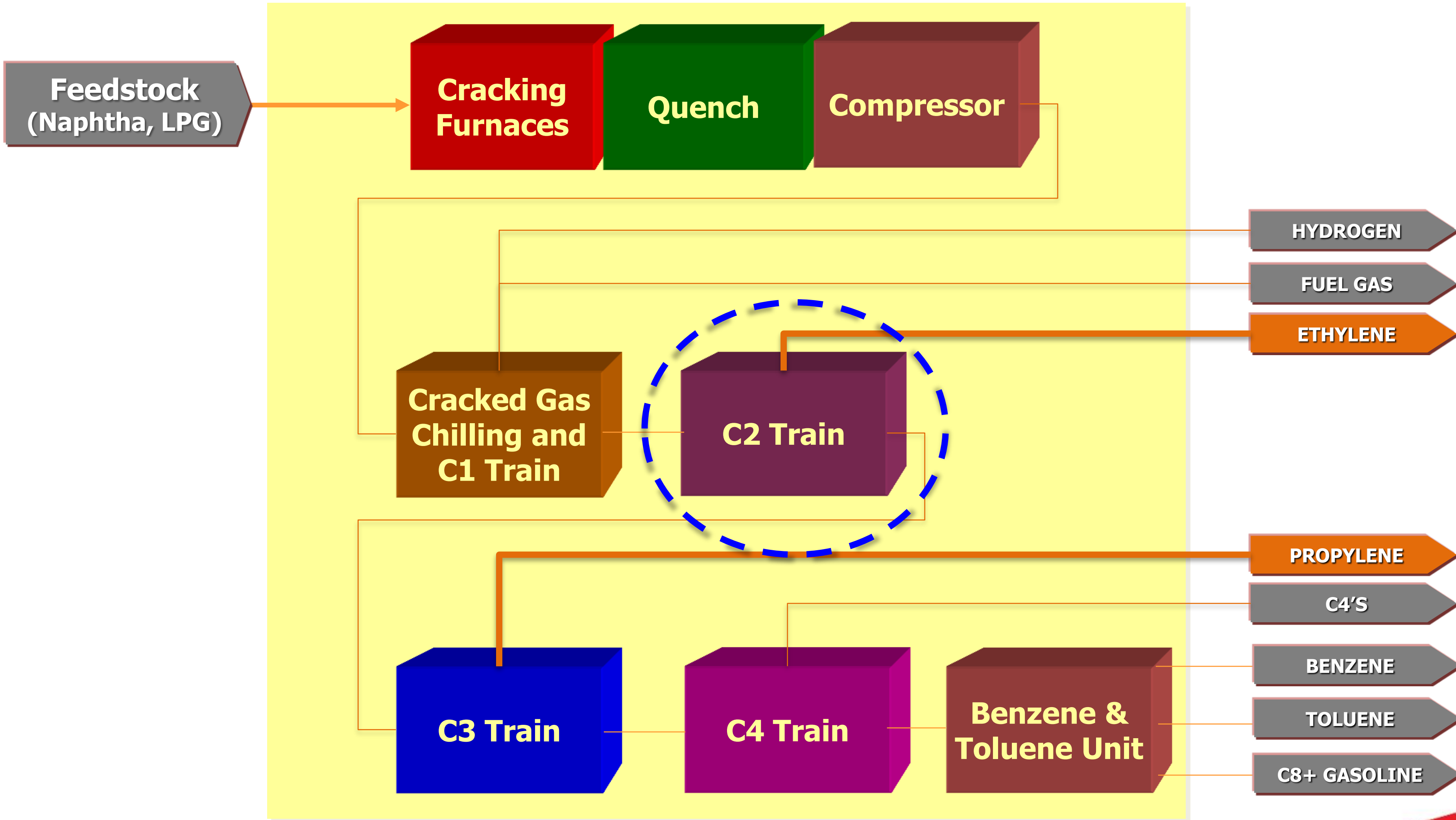
Intermediate
- PTA
- MMA
- EDC/VCM
- Styrene

Downstream
- Polyethylene
- Polypropylene
- PVC
- PET
- Polystyrene
- Compound-PE/PP/PVC

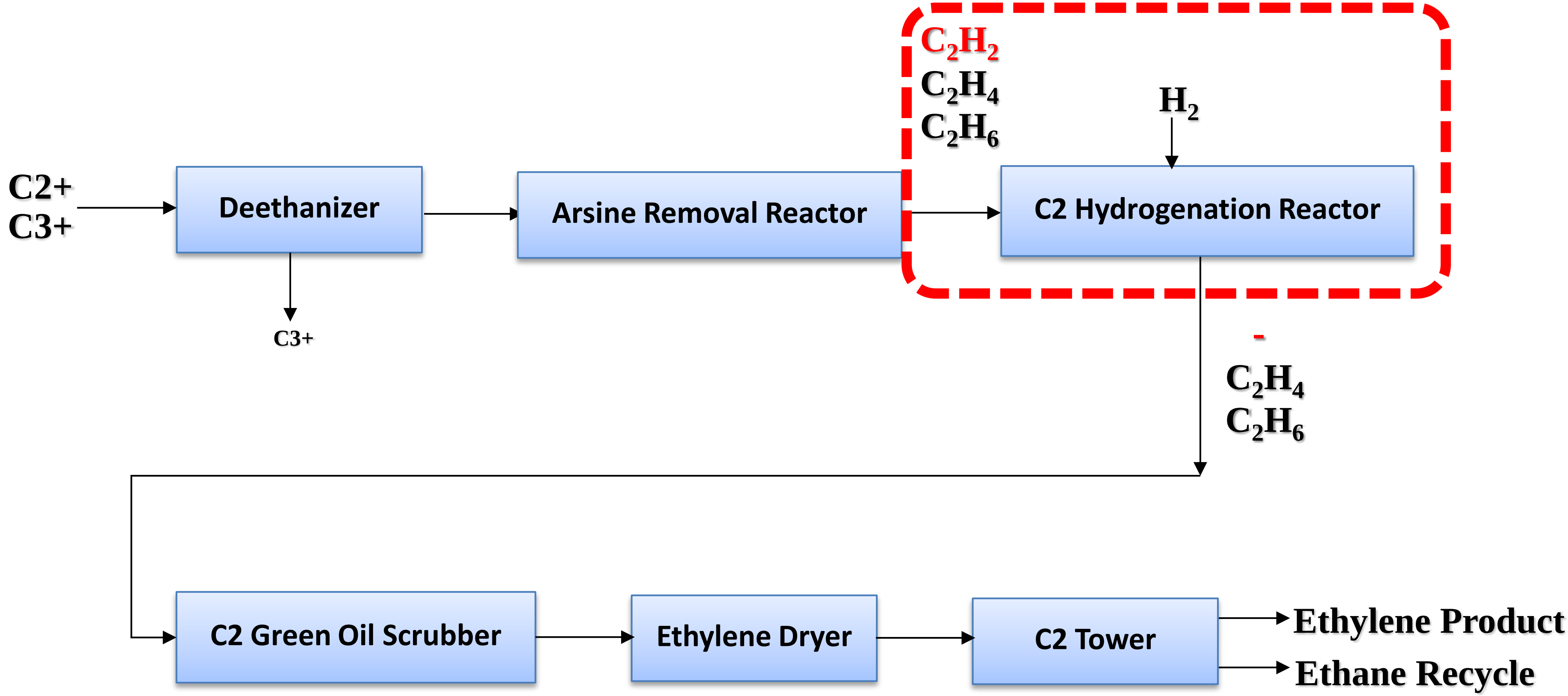
Converter
- Pipe & Profile
- Acrylic cast sheet
- Specialty films

2. Motivation and Objective

INTRODUCTION – Olefins Production Process

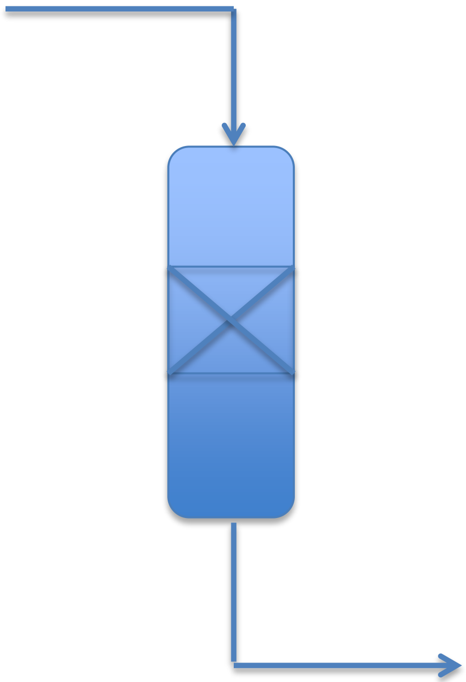


INTRODUCTION – C2 Train



Acetylene Hydrogenation Reactor (C2 Reactor) converts Acetylene (C_2H_2) to Ethylene (C_2H_4). However, undesired reactions could generate Ethane (C_2H_6) and Green Oil.

Acetylene
Hydrogen



Ethylene
Ethane
Green Oil

Main Reaction:

Desired reaction

- $C_2H_2 + H_2 \rightarrow C_2H_4$ — Acetylene hydrogenation → ethylene gain

Undesired reaction

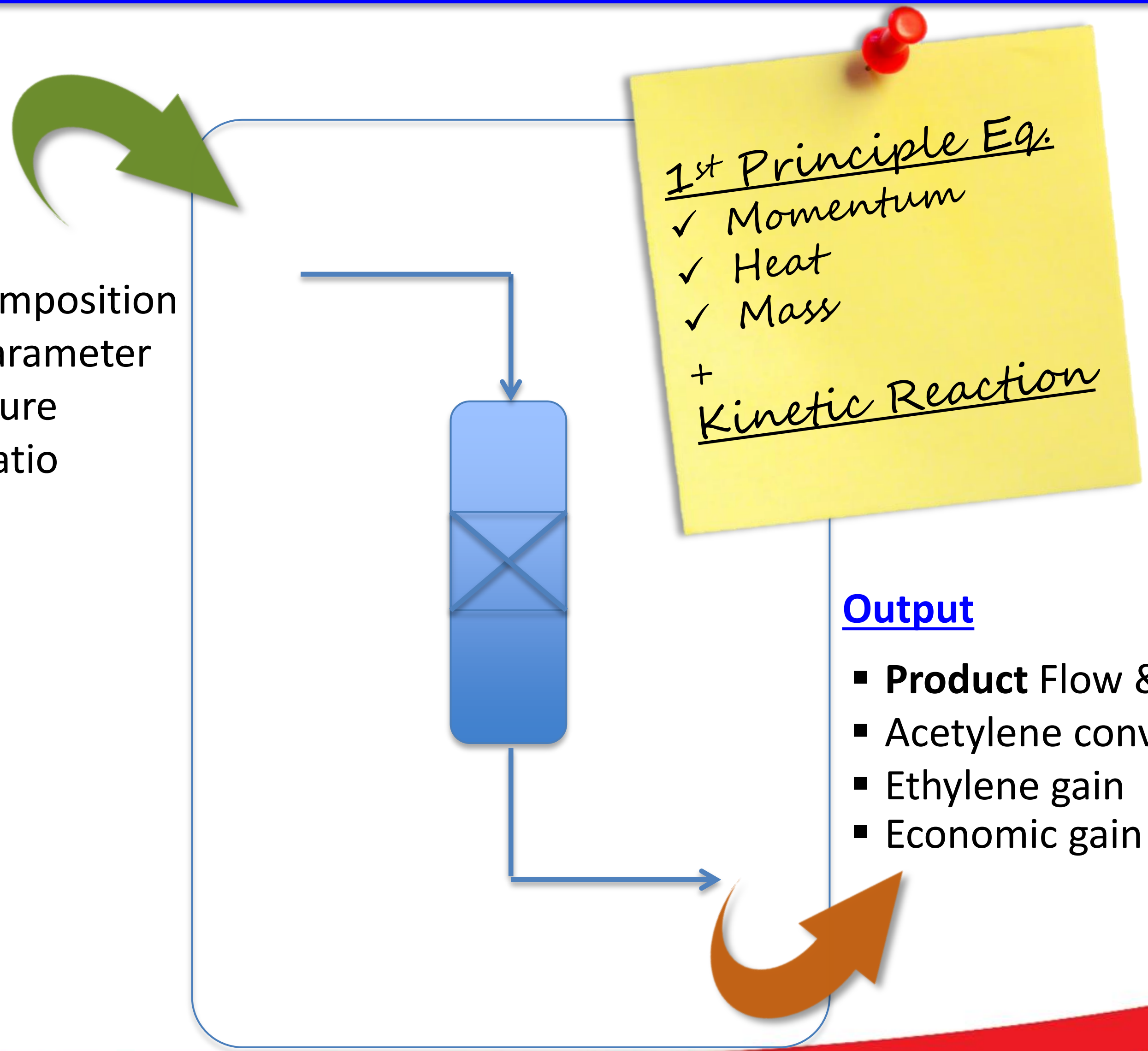
- $C_2H_4 + H_2 \rightarrow C_2H_6$ — Ethane hydrogenation → ethylene loss
- $2C_2H_2 + xH_2 \rightarrow C_4H_{4+2x}$ — Green Oil formation (Catalyst Decomposition)

Target: Max. Ethylene Gain
(Selectivity to Ethylene)

Detail Catalytic Reactor Model was developed using gPROMS Advanced Model Library for Fixed Bed Catalytic Reactors with detailed kinetic mechanism

Input

- **Feed** Flow & Composition
- **Manipulated** parameter
    - Temperature
    - H_2/C_2H_2 ratio



Output

- **Product** Flow & Composition
- Acetylene conversion
- Ethylene gain
- Economic gain

3. Methodology for Model Development

SCG’s C2 reactor model setup

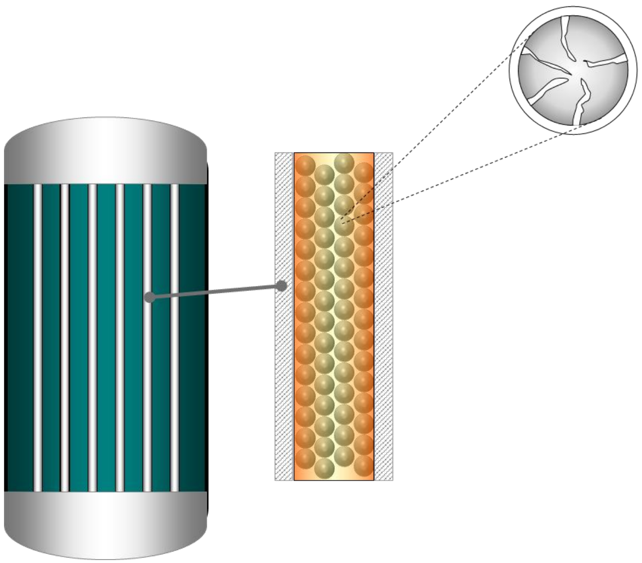
Fixed-Bed Catalytic Reactors (FBCRs):

Key engineering problems

1. **Scale-up**
   - Laboratory → Pilot → Commercial Plant
   - Maintenance of performance over scales
   - Cost efficiency in investment and operation
2. **Thermal stability – elimination of hot spots**
   - adjustment of catalytic bed properties – length, activity, shape of particles, etc
   - design of cooling system
3. **Catalyst lifetime**
   - Management of catalyst de-activation over operational cycle

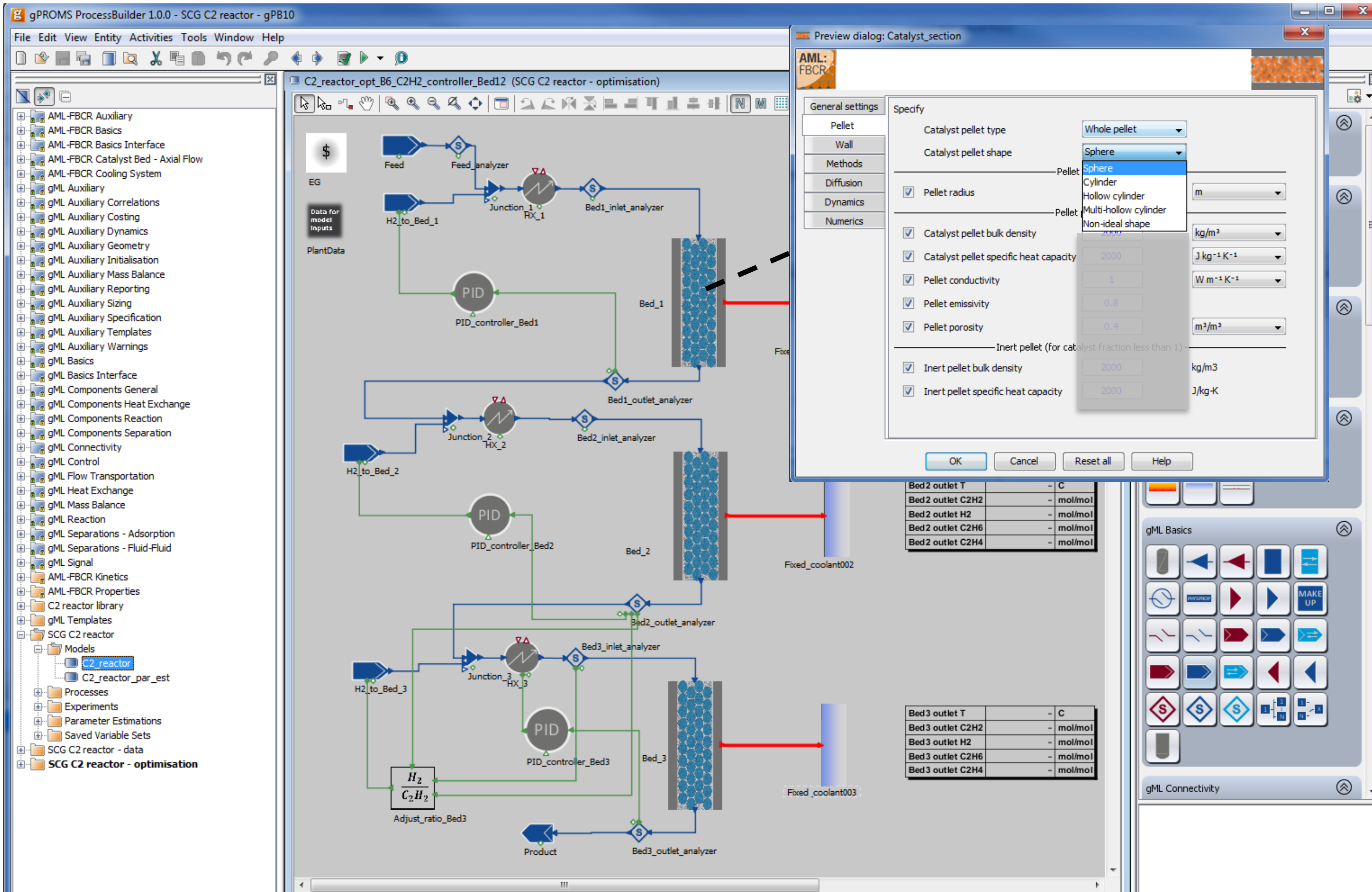
FBCR model-based analysis & design

- Requires high-fidelity models for
  - Catalyst particles
  - Tube
  - Shell side hydrodynamics (for multitubular reactors)



➔ gPROMS Advanced Model Library for Fixed-Bed Catalytic Reactors (AML:FBCR)

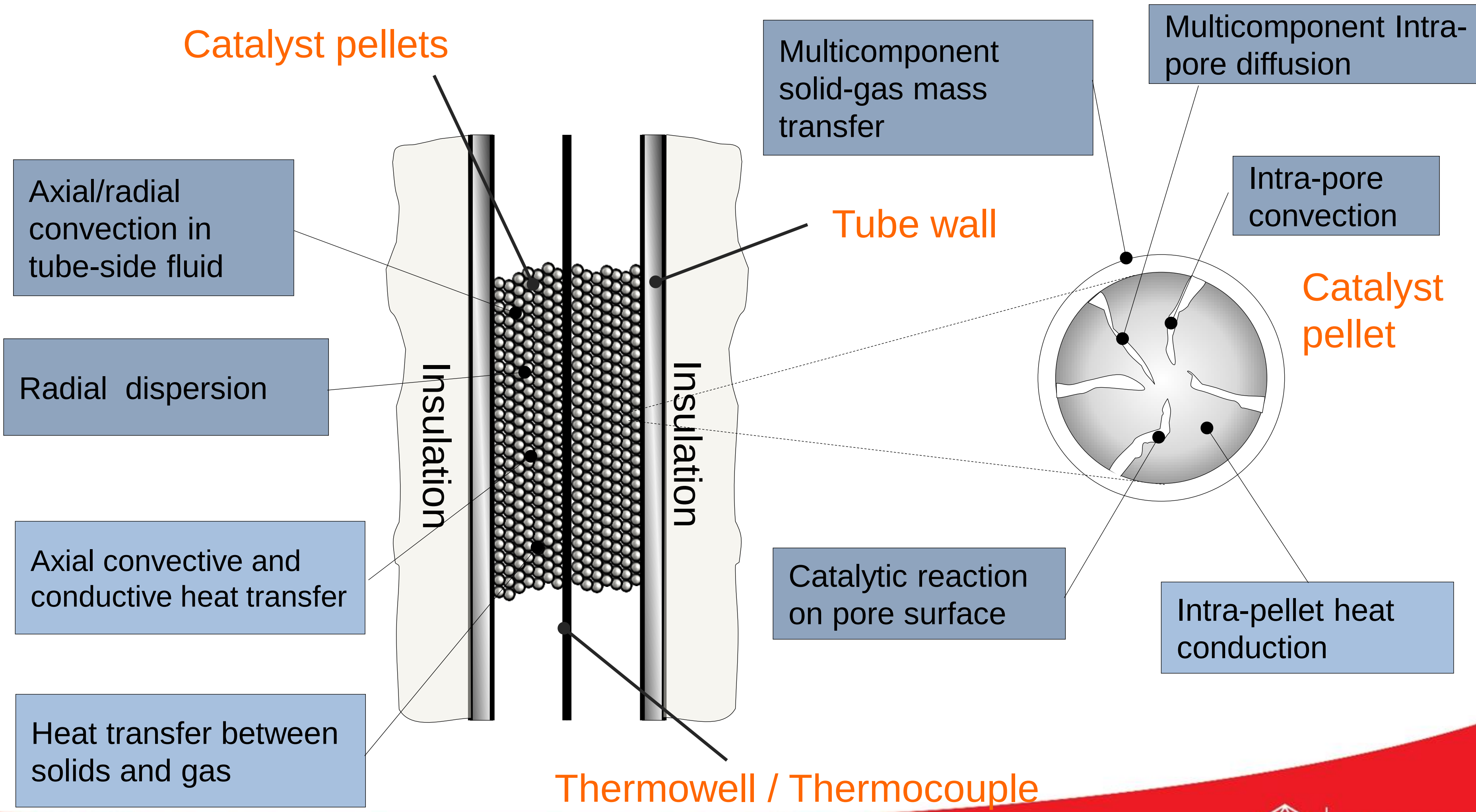
SCG's C2 reactor model in gPROMS ProcessBuilder



AML:FBCR overview

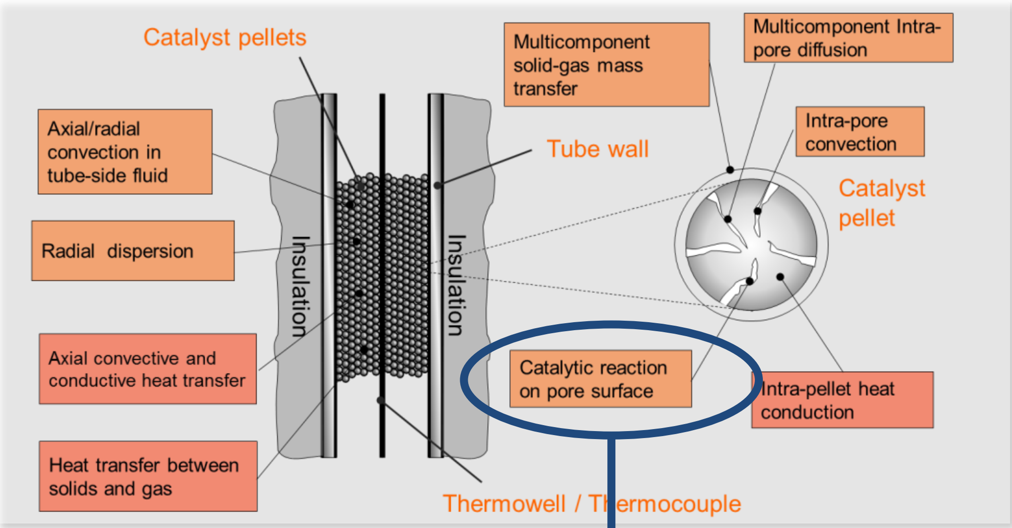
(for adiabatic reactors)

- Mass&heat transport and reaction phenomena



AML:FBCR overview

(for adiabatic reactors)



→ Comprehensive FBCR Model … combined with experimental data from lab, pilot plant, **commercial plant**

- Kinetic parameters cannot be derived from first principles
  - different from one catalyst to another

⇒ Need to be estimated from experimental data

3. Methodology for Model Development

Kinetic model development:
From plant data and literature to
an useful model

Determination of reaction kinetics: Main challenges

- Lab/pilot scale experiments are very important for deriving reaction kinetic mechanism for any catalytic reactions
(plant data typically do not have sufficient variability in operation conditions)

- How to derive complex reaction kinetics without small-scale experimentation?

→ Detailed **model-based analysis of historical data** taking account of most relevant hints from literature

→ Parameter **estimation of limited set of kinetic parameters** using historical plant data

→ Obtained model has limited predictive capability outside current range of operation conditions, but…
still **useful for identifying optimal operating strategy**

Acetylene hydrogenation reaction background (1)

- Borodzinski & Bond, Catalysis reviews 48, 2006

> importance. Ethene adsorption and the detailed mechanism of its hydrogenation on metal surfaces is still one of the most widely studied and debated problems in catalysis. The great complexities of hydrogenation of ethyne/ethene mixtures over palladium catalysts is the reason for slow progress in establishing a molecular mechanism for the process, and the nature and the types of active site. The role of carbonaceous species adsorbed on metal

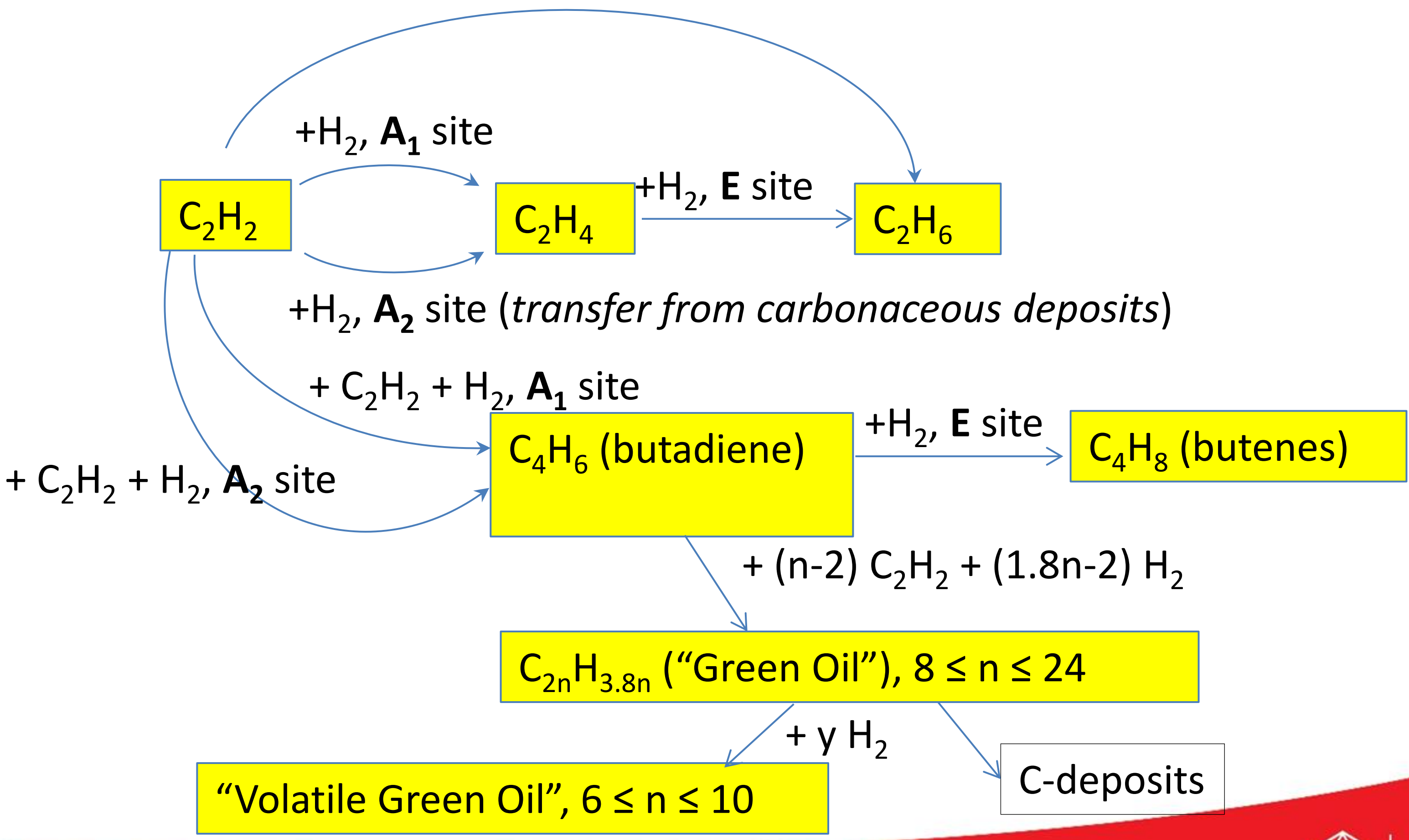
- Key aspects to be considered in C2 reactor hydrogenation kinetic model

1. Acetylene and Ethylene hydrogenation reaction
   - Different catalyst active sites for acetylene and for ethylene hydrogenation
   - Reaction mechanism known to depend on reaction conditions (high v. low acetylene concentrations)
2. C4s formation (Acetylene dimerization)
3. C6+ and Green oil formation (Acetylene hydro-oligomerization)
4. Catalyst deactivation during run (loss of activity)
5. Selectivity change during run (loss of selectivity)
6. Irreversible activity loss due to catalyst regeneration cycles

None of the published literature capture sufficiently catalyst deactivation and loss of selectivity

Acetylene hydrogenation reaction background (2)

- Example of reaction scheme formulation based on literature:

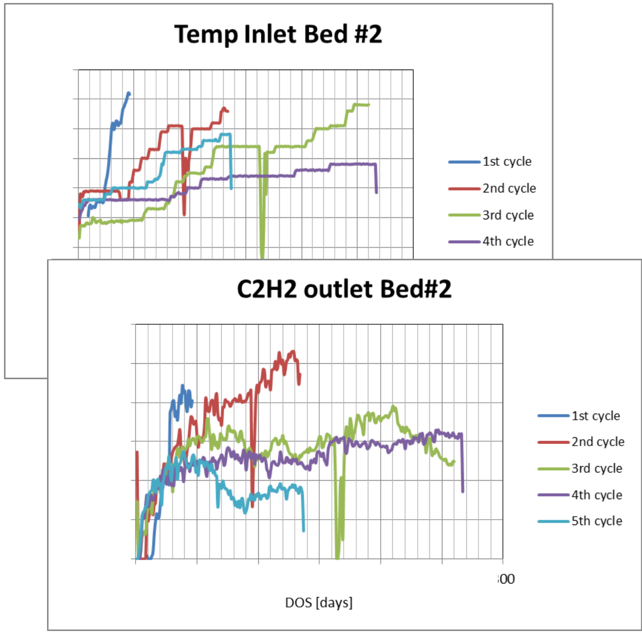


Reaction scheme formulation for SCG's reactor model

- Reaction scheme need to be based on components which are measured
- No way to distinguish between parallel reactions on different active sites

Estimation of kinetic parameters

- Data from 6 historical cycles were processed and included in gPROMS ProcessBuilder
- Controls included time profiles of:
  - Feed rate, feed composition and pressure
  - Inlet temperature and H_2 flow to each bed
- Measured data included time profiles of:
  - C_2H_2 and H_2 concentrations at outlet from each bed
  - Temperature measurements at outlet and inside each bed
  - C_4s and C_6s product flowrates from recent cycle

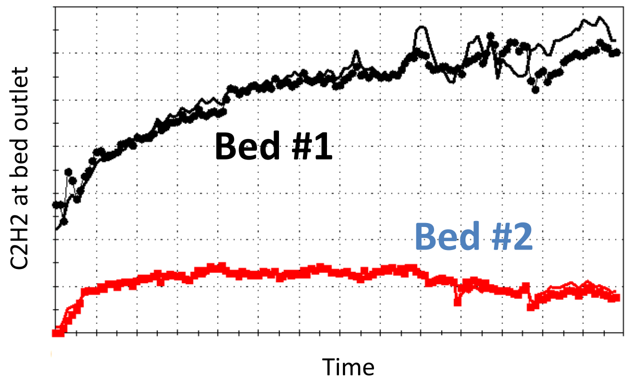


→ Estimated >20 kinetic parameters, bed 3 with different kinetic mechanism than beds 1&2

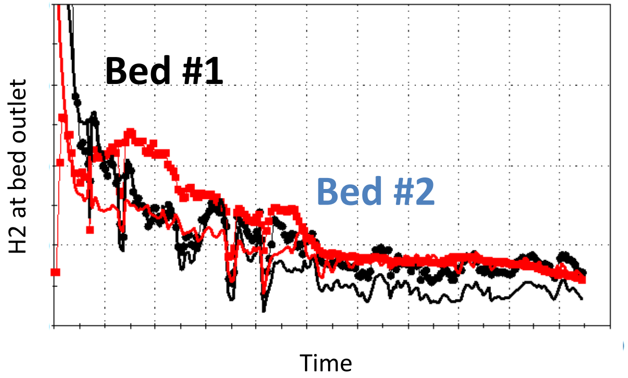
→ Plant data from historical cycles reproduced by the model reasonably well

Typical fit to historical plant data

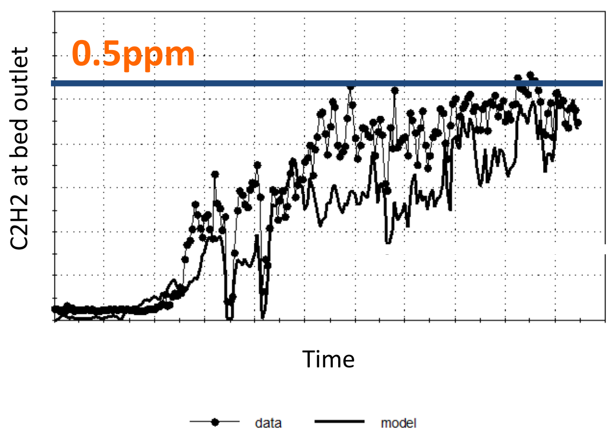
C_2H_2



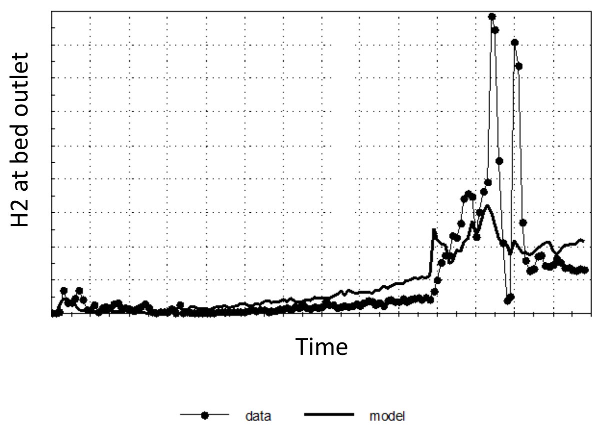
H_2



Bed #3



Bed #3



3. Methodology for Model Development

Optimisation of C2 reactor operation

Optimisation problem setup

- Objective function: Economic gain from C2 reactor

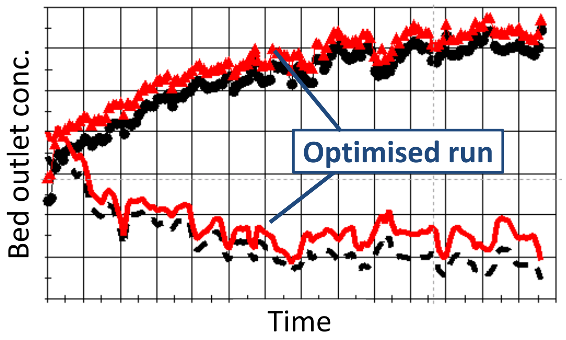
Economic Gain = Diff. Variable Cost – Fixed Cost

- Diff. Variable Cost = More Ethylene Generated – Less H2 Consumed
- Fixed Cost = Regeneration Cost + Switching Cost + Catalyst Depre. Cost

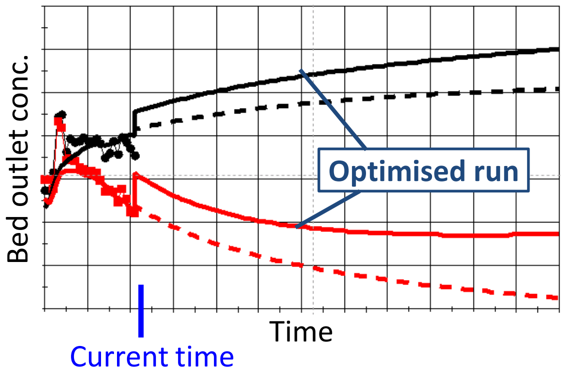
- Decision variables
  - Run length
  - Time-varying controls over run length
    - Inlet temperature to each bed
    - H_2 flow to each bed
- Constraints
  - Maximum bed temperatures
  - Outlet C_2H_2 concentration

Optimisation approach

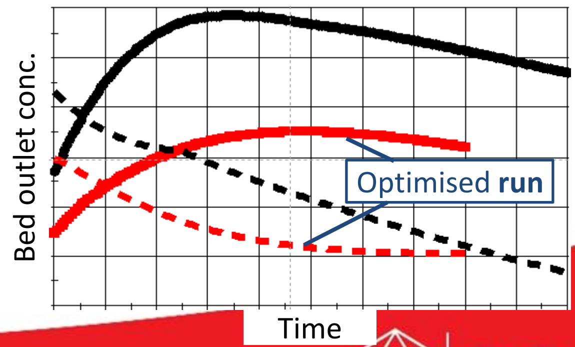
A. Demonstration on historical cycles
- Inputs read from data (flowrate, feed composition, pressure)
- Controls optimised for whole run



B. Optimisation of current cycle
- Inputs read from data until current date, then assumed
- Controls optimised from current time onwards



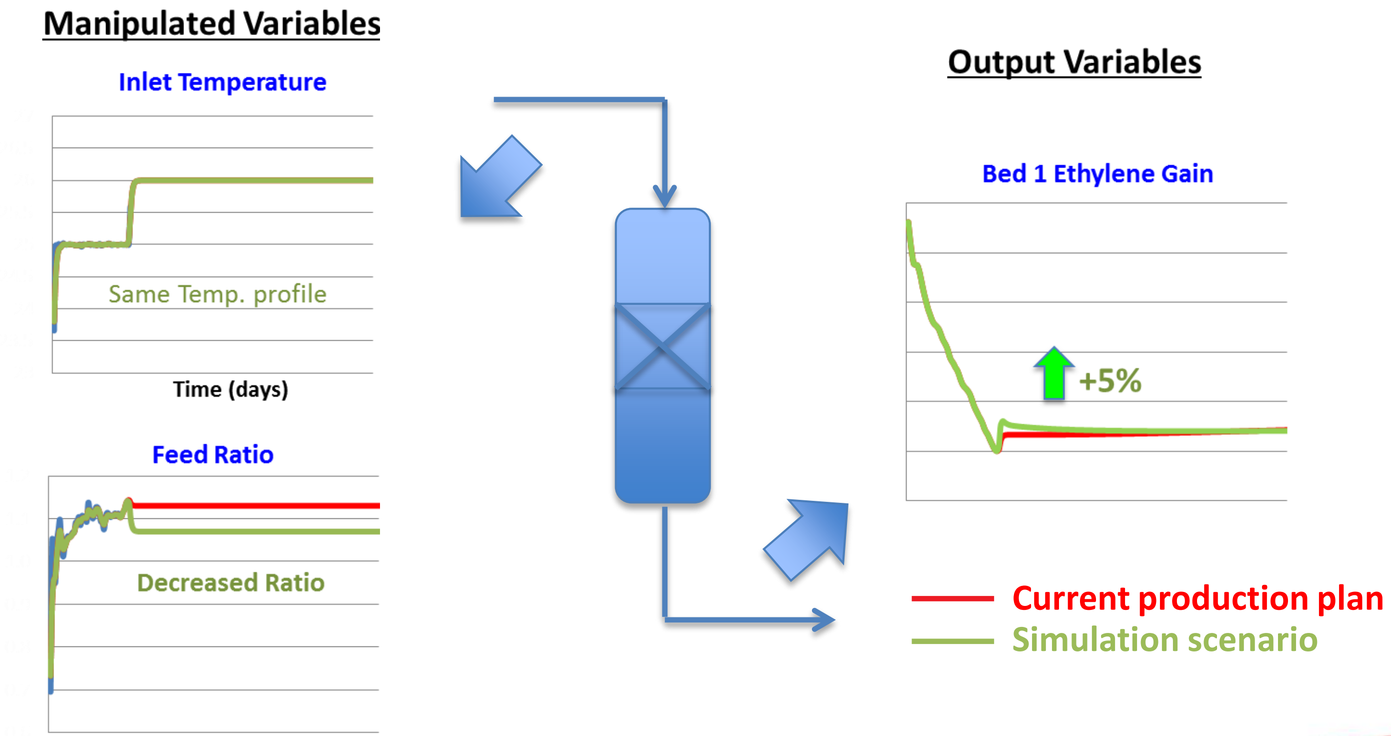
C. Optimisation of new cycle
- Inputs assumed
- Controls optimised during whole run



4. Applications / Benefits / Summary

The Model can be used to simulate a scenario before adjusting real process parameters

- Benefits of Simulation scenario
  - ✓ Weekly production planning
  - ✓ Process condition improvement
  - ✓ Process risk assessment

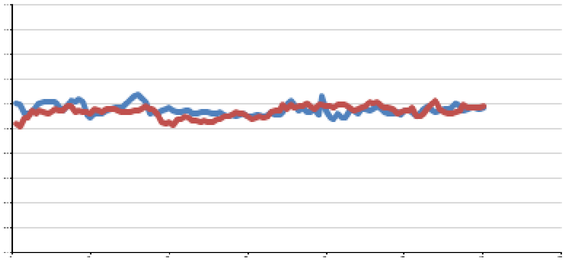


Optimization Case … Suggest the new operating policy for improved benefit.

New Operating Policy

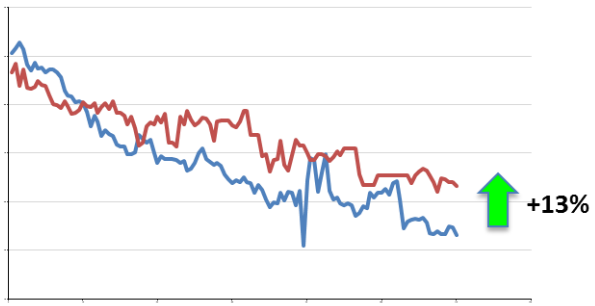
Inlet Temperature

Feed Ratio

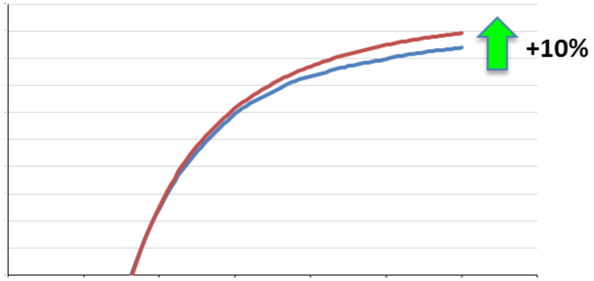


Model Outcome

Ethylene gain (%)



Economic gain (M$/y)



SUMMARY

- A rigorous model of acetylene hydrogenation reactor is successfully developed on gPROMS ProcessBuilder

- The model is capable of explaining the reactor behavior and suggesting new operating policy
  - Prediction: Product Stream, Outlet Conditions and Catalyst Performance
  - Optimization: Optimum temperature, feed ratio and run length
  - Benefit: Improve economic gain significantly!!!

- Knowledge and model can be applied to other fixed bed reactors

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THANK YOU