Advanced Process Modelling: A 21st century paradigm for lasting process improvements

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Agenda

- PSE at a glance
- Advanced Process Modelling
- Some application examples in the petrochemical industry
- Conclusion
1989 – 1997

Company ‘spun out’
Acquires gPROMS® technology

100s of person-years of R&D with industry

1997

Private, independent company incorporated in UK

Royal Academy MacRobert Award 2007 for Engineering Innovation

2011

- Software and advanced services (60:40)
- Major process industry focus
- Driven by R&D and Innovation; gPROMS now in 4th generation
- Financially independent
- Worldwide operations

London HQ
Germany
Korea
Japan
USA
Saudi Arabia
India
Thailand
A **multipurpose** advanced process modelling environment that combines
- Custom equation-based modelling
- “Drag-and-drop” flowsheeting

**Equation-based, open** models
- Transparency, maintainability
- Simulation
- Optimisation
- Parameter Estimation
- Experiment Design

...**steady-state or dynamic**

World’s most advanced **solution engine**
- Integral & Partial Differential and Algebraic Equations (IPDAEs)
- Handling of extreme **model discontinuities**
- Integrated combined symbolic & numerical computation
- Solves models with hundreds of thousands of equations

**Open software architecture**
- Embed gPROMS inside 3\textsuperscript{rd} party software
- Embed 3\textsuperscript{rd} party software inside gPROMS
PSE’s market space: the process industries

**Americas**
- Air Products • BP Chemicals
- Carus Corporation
- CD Tech • C&I Engineering
- Dow Chemicals • DuPont
- ExxonMobil • Ineos
- Praxair

**EMEA**
- Arkema
- BP Exploration • BASF • CEPSA
- Infineum • Indorama
- Jacobs Engineering
- Linde • Morgan Stanley
- Plaxica • Repsol • SABIC
- Sasol • Shell
- Süd-Chemie • Sulzer
- TOTAL • Wacker Chemie
- Wolff Cellulosics

**APAC**
- Idemitsu Petrochemicals
- GS E&C • Hyosung
- JGC • LG Chem
- Mitsubishi Chemical
- Posco • Samnam Petrochemical
- SKC • SK Chemicals
- SK Energy
- SK Petrochemicals
- Taiyo Nippon Sanso

**Energy Solutions**
- Folgers
- Johns Manville
- Minera EXAR
- Procter & Gamble
- Pfizer • SQM
- Toyota Motor US
- United Technologies RC
- United Technologies Power

**Other**
- Anglo Platinum • Atomic Weapons Establishment
- Cadbury’s • Ceres Power
- det Norske Veritas
- FL Smidth • Friesland Foods
- National Nuclear Labs
- Nestlé • Purac
- RWEnpower • Tetrapak
- Topsøe Fuel Cells
- Veolia • Voith Paper

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Advanced process modelling
Rationale for advanced process modelling

- **21st century methodology for design, optimisation and control** of chemical processes;
  - Use expanded due to availability of highspeed computers and software packages;
  - Existing approaches are sequential methodologies going back to 1970’s and 1980’s

- **Integration of process value chains**
  - Lasting business value and competitive advantage stem from integral margin optimisation of evolving and changing process value chains

- **Search for operational excellence**
  - OEE – Operational Equipment Excellence (Loading, Availability/Uptime, Performance, First run through quality)

- **Crystal ball capability (really?)**
  - Sound understanding of engineering and mathematical fundamentals (physical system and chemistry); process cannot be viewed as a black box
  - **Integrated and simultaneous** application of physical, chemical and business relationships
  - Model validation and knowledge of uncertainties
... While there are always lots of uncertainties, the key challenge in engineering is to find those problem components that contribute most to uncertainties in outcomes ...
Three dimensions of Advanced Process Modelling

I. Scope

1. Catalyst particle
2. Sub-unit
3. Equipment unit
4. Process plant
5. Intra/inter-organisational supply chains
6. Product end-use & function
Three dimensions of process modelling
II. Model detail

Lumped models → 1d models → 2d models → 3d models → 4+ d models

- Log-continuous distribution of Paraffins C6 +
Three dimensions of process modelling

III. Process lifecycle application

**R & D**
- Laboratory data analysis
- Optimal experiment design
- Conceptual process design
- Catalyst design and analysis

**Engineering design**
- Process front-end design (FEED)
- Detailed design of key units

**Operations**
- Process and equipment design optimization
- Control design and verification
- Design of optimal operating procedures
- Online Model-Based Applications
- Troubleshooting with detailed predictive models

Optimal experiment design

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Advanced Process Modelling – the drivers

Leverage modelling investment across process lifecycle.

- minimal cost of model development & maintenance, consistency throughout

Use validated models that are predictive over wide ranges of design & operating parameters

→ reduced risk in innovation and operations

Capture all important interactions

→ meaningful engineering objectives
Some application examples in the petrochemical industry

Hunt refining company – Dimethylsulfide reactor
Repsol – HPPO process development
Süd-Chemie – Optimizing Methanol Synthesis
[Undisclosed] – PTA oxidation reactor optimisation (hybrid gPROMS – CFD modelling)

... also model-based control based on first principles models; multi-period, multi-site supply chain optimisation; state estimator based scenario prediction
July 2010, Tuscaloosa, Alabama (US)

DMS process technology : Gaylord Chemicals
Reactor design : PSE
Reactor manufacture : DWE
Operator : Hunt Refining

Key points:  
- Uncertainty of inputs; yet, strict product quality required  
- Catalyst variability and lifetime optimisation

HPPO Process Development

HPPO: Hydrogen Peroxide route to Propylene Oxide

\[ \text{CH}_3\text{CH}=\text{CH}_2 + \text{H}_2\text{O}_2 \rightarrow \text{CH}_3\text{-CH-CH}_2 + \text{H}_2\text{O} \]

- **HPPO process**
  - addresses problems with conventional process
    - no SM co-product
    - minimal by-products

- **Joint REPSOL/PSE project**

- December 2010
  Plant Design Special Issue
  H. Martín Rodríguez, A. Cano, M. Matzopoulos
Identification of key process parameters
Model-based analysis of experimental data

- Single-tube pilot reactor
  - well-cooled (“isothermal”)
- Detailed model of experimental rig
  1. perform parameter estimation
  2. assess parameter accuracy
  3. design subsequent experiments
- Two-step identification
  - reaction kinetics parameters
  - heat transfer parameters
- Minimum number of experiments

Obtain optimal estimates of model parameters, correlation and of their accuracy

 Quantify uncertainty in model-based decisions

-> MANAGE RISK in TECHNOLOGICAL INNOVATION and PROCESS DEVELOPMENT/OPTIMISATION

Source: H. Martín Rodríguez et al., Hydrocarbon Processing, Dec-2010
Objective
- minimise total annualised cost of production
  - combined CAPEX/OPEX

Constraints
- quality constraints on product
  - maximum ppm levels of several impurities
- safety constraints
- coolant supply and return temperature constraints
- effluent concentration constraints
- reactor shell-side velocity constraints (to prevent tube fouling and excessive vibration)
- reactor and column dimensions

SIMULTANEOUS DESIGN APPROACH
1. Consider whole plant simultaneously

2. Use detailed equipment models to ensure design
  - reflects true process economics
  - satisfies all important constraints

3. Apply rigorous mathematical optimisation
  - too many decisions for trial-and-error simulation!
  - 49 continuous & discrete decisions “MIXED INTEGER OPTIMISATION”

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Process design
1. Reactor

- Liquid-phase exothermic
  - Multitubular equipment

- Design decisions
  1. Number of active reactors?
  2. Tube length/diameter?
  3. Tube pitch (relative to tube O.D.)?
  4. Number of baffles?

- Operational decisions
  5. Mass fraction of $H_2O_2$ in feed?
  6. Molar ratio of PP to $H_2O_2$ in feed?
  7. Process stream inlet flowrate/temperature?
  8. Cooling water inlet flowrate/temperature?
  9. . . . . . . . . . . . . . . . . . . . . . . . . . . . .

Source: H. Martín Rodríguez et al., Hydrocarbon Processing, Dec-2010
Process design

2. Separation section

- Complex separation
  - large number of columns
  - two columns with chemical reaction
  - one azeotropic distillation
  - 25 components (reactants, solvent, product, byproducts, impurities)

- Column design decisions
  - no. trays, feed tray position
  - diameter

- Column operational decisions
  - reflux ratio, reboil rate
  - pressure

Source: H. Martín Rodríguez et al., Hydrocarbon Processing, Dec-2010
3. Overall process

- Many possible separation section structures
  - are all these columns really necessary?
  - Robustness of design and process controllability

- 2 significant recycles
  → tightly coupled reaction & separation with multiple design, engineering and financial constraints

- Key results
  - 2 columns eliminated entirely → saved tens of millions of €/year compared to Base Design
  - Financial constraints met (IRR); in contrast, traditional and sequential design process failed

Source: H. Martín Rodríguez et al., Hydrocarbon Processing, Dec-2010
Customized Synthesis Loop Models
Plant with Steam Reformer, Add. Feed, Real Circulator, LP Separator, Hydrogen Recycle

Source: Seuffert et al., PSE Advanced Process Modelling Forum 2012
Optimizing Methanol Synthesis (2)
From Lab to Industrial Plants via High-Fidelity Modeling

Source: Seuffert et al., PSE Advanced Process Modelling Forum 2012
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Optimizing Methanol Synthesis (3)
From Lab to Industrial Plants via High-Fidelity Modeling

- **Accurate** prediction of catalyst de-activation vs. cumulative production for both reactors

Source: Bäumler et al., PSE Annual Meeting 2007

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Hybrid gPROMS/CFD equipment modelling

Concept: combine *different* descriptions of processing equipment within *single, fully coupled* model

Computational Fluid Dynamics (CFD)
- Fluid mechanics (single/multiphase)
- Mixing

gPROMS
- Heterogeneous reaction
- Heat & mass transfer
- Nucleation & growth
- Electrochemistry
Example
Gas/liquid/solid reactors for PTA

Model accurate enough to identify improvements in raw material consumption of ~1% confirmed by actual plant implementation
PSE’s modelling approach

Detailed reactor hydrodynamics

- Hybrid Multizonal gPROMS/CFD Model
  - Unique, proprietary PSE technology

- Detailed hydrodynamic description
  - $k$-$\varepsilon$ turbulence model
  - Multiple Reference Approach (MRF) for impeller modelling
  - Eulerian-Eulerian two fluid model
  - Schiller and Naumann drag model
    - implemented via UDF

- ...all combined with full descriptions of thermodynamics, kinetics, gas/liquid mass transfer
  - ➔ much more powerful than “pure” CFD analysis
Plant revamp studies

Feed and product withdrawal locations
Internals design, layout and geometry
Operating conditions
Key phenomena modelled: Reaction, hydrodynamics, crystallisation

Impeller type and spacing

PSE & client jointly determine possible alternative reactor configurations to be evaluated to identify the optimal internal configuration
Plant revamp
Example: 4 reactor design alternatives
Results: Sauter mean bubble diameter and volume specific power input

Alternative 1: Concave impeller exhibits highest dissipation

Alternative 2: Hydrofoil exhibits lowest dissipation

Alternative 2 exhibits far larger bubbles than the other alternatives → Lower surface area in middle section.
Performance of alternative reactor configurations

- **Alternative 2** is optimal one
  - reduction in raw material consumption
  - savings of $3.6/tonne TA

- If Alternative 2 is modified to use a **single bottom reflux nozzle**, then the additional expected reduction in raw material cost will be in the order of $3.1/tonne TA

- Final selection not dictated by largest reduction in raw material cost, but by best financial metric (e.g. RONA)
Conclusions

- Advanced Process Modelling (APM) is an industry tested and proven paradigm for the 21\textsuperscript{st} century
  - Software technology has advanced tremendously in the last 10 years if based on modern software engineering concepts
  - All process lifecycle requirements are now available with a single technology approach and integrated in a single calculation
  - Model validation and predictability

- APM integrates rigorous mathematics with uncertainty principles
  - Probability outcome
  - Scenario analyses

- Advanced skill set is required (mathematics, engineering principles) \(\rightarrow\) industry recognises need
Thank you!

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