Developing inferentials based on Digital Twins: Distillation case studies

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• Who we are
• I don’t want to believe: Analyzer vs. Peng-Robinson
• Our Lifecycle Digital Twin vision
• Developing Inferentials with Digital Twins
• Customer Case Studies in distillation
• Your takeaways, Q&A
Who we are
Inprocess: 1-slide Introduction

Since 2006 helping the processing industries in solving design and operational issues

**Inprocess Solutions & Services**

- **2006**: est. in Barcelona by domain experts
- **55 countries**: worldwide presence
- **60+**: simulation engineers
- **380+**: executed projects
- **330+**: training courses

**inprocess**

- independent from any provider (process simulator or ICSS)
- our core business is Process Simulation
- enthusiastic about sharing its knowledge with our clients

**Lifecycle Modelling and Operator Training Simulators**

**Process Simulation Studies**

**Professional Development & Training**

**Applications and Software Products**

Since 2006 helping the processing industries in solving design and operational issues.
Science is built on proven laws. There is not option to don’t believe them.

Process Simulation is not a question of believing or not

Strangely enough, plants are following those laws
In 1976, Dr. D. Robinson and Dr. Ding-Yu Peng developed the Peng-Robinson Equation of State. EoS equations are used in simulators to calculate Vapor-Liquid equilibrium of mixtures of hydrocarbons.

Online Analyzers require a proper maintenance and regular calibration to produce reliable results.

We use them to control the plant

We use them to design the plant
Our Lifecyle Digital Twin vision

Also called:

LifeCycle Operator Training Simulator (LC OTS)

Or

Multi-Purpose Dynamic Simulator (MPDS)
Digital Twins are virtual copies of physical assets and their operating behaviours.

This definition has several points of view which are complementary to each:

- Mechanical and structure models
- Contextualized 3D models
- Empirical Models (data fitting)
- First-Principles Models

Centuries of Physics, Chemistry and Thermodynamics knowledge are consolidated here!
The Process Digital Twin is a first-principles steady-state or dynamic simulation model that contains:

- all the process layout and streams conditions (Compositions, Pressure, Temperature, Flow, etc);
- all the equipment geometric data (dimensions, elevation, tray sizing, sensor location, etc);
- all equipment manufacturer performance data (pump curves, compressor curves, heat exchanger rating data, etc);
- all actuated valves (valve pressure drop, sizing, characteristic, etc);
- and all the control and instrumentation (control loops, PID algorithms, instrument ranges, tuning constants, etc).

All this information is combined in a Process Model, built in a high-fidelity simulation tool like Aspen HYSYS. Depending on the purpose, it can be Steady State or Dynamic.
Lifecycle Process Digital Twin

Plant lifecycle

Conceptual Design → Basic Design → Detailed Design → Set-up → Commissioning → Operation → Maintenance and Modernization

1. Design Simulation
2. Virtual commissioning and simulation-based engineering
3. Operators Training
4. Operation-associated decision support and optimization

Off-line
- Engineering Design validation
- Control Narrative & Procedures validation
- ICSS validation & tuning
- Operator Training Simulators (OTS)

On-Line
- Equipment Load & Efficiency Monitoring
- Inferentials
- Bad Actors Detection
- Look-ahead & What-if

First-Principles Models

IIS

Communication

Sensors Data

CLOUD DATABASE

ASSET
Developing Inferentials with Digital Twins
Finding the Truth with Industrial HI (Human Intelligence)

The Process Data
Plant sensors provide vast data sets of what is “Out There”. With the right visualization tool an experienced eye can make clever use of it.

The Laws
Hundreds of “Data Scientists” worked hard along the centuries to discover the laws of how matter behaves. Those laws still last today.

The Calculator
Process simulation is only a macro-compiled code of physics, chemistry and thermodynamics laws smartly coded in an interactive computer application.

Industrial Human Intelligence

The Engineer
A combination of skills in chemical engineering, process control, plant operation coupled with plant data visualization, process simulation, programming and some common sense.

The Truth
Building distillation Inferentials with HYSYS

**Known Thermo?**

- NO: Forget it
- YES:
  - **Binary mixture?**
    - YES: Simple HYSYS Steady-State
    - NO:
      - Dynamic effects?
        - NO: Column HYSYS Steady-State
        - YES: Column HYSYS Dynamics
  - Dynamic effects?
    - YES: Column HYSYS Dynamics
    - NO:
      - Dynamic effects?
        - YES: Column HYSYS Dynamics
        - NO: Column HYSYS Steady-State

**Explicit Algebraic Formula for AspenIQ or DCS calc.**

\[ \text{Example Formula} = a + b\cdot V_1 + c\cdot V_2 + d\cdot V_1^2 + e\cdot V_2^2 + f\cdot V_1\cdot V_2 \]

- \( a = -124.125 \)
- \( b = -1.7447543 \)
- \( c = 7.8426775 \)
- \( d = -0.00104104771 \)
- \( e = -0.06703829112 \)
- \( f = 0.02494089626 \)

**Correlation Coeff. (r):** 0.9971

**Online IIS + HYSYS Dynamics**

- Configure IIS app and deploy
- Customer RTDB: Aspen IP21, OSI PI, CDF
- IIS: Online IIS + HYSYS Dynamics
- No Feasible regression
## Building distillation Inferentials with HYSYS

<table>
<thead>
<tr>
<th>HYSYS case</th>
<th>Method</th>
<th>Deliverable</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple HYSYS case</td>
<td>Develop Multi-case study and correlation</td>
<td>Report with Explicit Algebraic Formula</td>
<td>2-3 days</td>
</tr>
<tr>
<td>Calibrated column with HYSYS Steady-State</td>
<td>Develop Multi-case study and correlation</td>
<td>Report with Explicit Algebraic Formula</td>
<td>2-3 weeks</td>
</tr>
<tr>
<td>Calibrated column with HYSYS Dynamic</td>
<td>Develop Multi-case study, generate raw data set and install application</td>
<td>Online IIS application with Lookup table or HYSYS Steady-State</td>
<td>3-4 weeks</td>
</tr>
<tr>
<td></td>
<td>Configure and install application</td>
<td>Online IIS application with HYSYS Dynamics runtime</td>
<td>4 weeks (model from OTS) or 8 weeks</td>
</tr>
</tbody>
</table>
Customer Case Studies in distillation
Case Study 1: C3= in Deethanizer bottoms

- For the APC controller of the downstream C3= Splitter it is important to infer the C3= content since it is an important FeedForward variable.
- Such an inferential can be calculated based on the Deethanizer bottoms conditions.
- HYSYS data was regressed to build an **Explicit Algebraic Formula**

**Unbiased** algebraic formula: C3= in DC2 bottom

**Back-Calculated C3= content** from downstream C3splitter. 1 month data.

2 hours anticipation

Inferential C3=
Case Study 2: C3= in C3Splitter bottoms

- C3\(^{=}\) content in C3splitter bottoms is measured by Online Analyzer every 15 min.
- An inferential can provide a value every minute without the Analyzer delay.
- HYSYS data was regressed to build an Explicit Algebraic Formula for the inferential

Online Analyzer C3\(^{=}\) content: 1 month data

Unbiased algebraic formula: C3\(^{=}\) in C3splitter bottom
Case Study 2: C3= in C3Splitter bottoms

- The inferential provides a 15 minutes advance and less damped signal over the Online Analyzer.
- It can also reveal when the Online Analyzer needs maintenance.
Case Study 3: Depropanizer bottoms

- The bottom of the column does not have an online analyzer. The DMCPlus cannot operate optimally if it does not have the bottom propane as a controlled variable.
- The main variables that affect the propane at the bottom are the equilibrium pressure and temperature, but also the C4s in the inlet.
- It was done in HYSYS a multiple 3-variable Case Study and fitted with a multivariable non-linear correlation in an Explicit Algebraic Formula.

HYSYS Model
- Matching plant data

Multiple Case Study
- 15k data points

Correlation
- Non linear Regression
  \[ R^2 = 0.99 \]
Case Study 3: Depropanizer bottoms

Propane Lab data: 9 months

HYSYS Multiple variable inferential

Basic inferential only with P and T

The graphic shows the unbiased inferential (just explicit formula without lab bias update)
Caprolactam content in column is sampled for LAB every 8 hours

HYSYS data was regressed to build an Explicit Algebraic Formula

Unbiased algebraic formula: Caprolactam % content

Column Bottom Temp

Column Bottom Pressure (90 to 130 mmHg absolute)

LAB Caprolactam % content

Unbiased algebraic formula with fix 12 mmHg correction factor on pressure variable
Case Study 5: Double C3Splitter, C3= in bottom

- C3= content in C3splitter bottoms is measured by a picky Online Analyzer.
- HYSYS data was regressed to build an **Explicit Algebraic Formula**

LAB sample C3= content. 1 year data.

**Unbiased** algebraic formula: C3= in C3Splitter bottom

Online Analyzer DESCALIBRATION
Case Study 5: Double C3Splitter, C3= in bottom

- The quality inferential was evaluated with a plant perturbation test. The inferential gave a 5 hour anticipation over the Online Analyzer.
- The Online Analyzer gives a false zero value out of the test.

Unbiased algebraic formula: C3= in C3Splitter bottom

Online Analyzer C3= content
Case Study 6: Double C3Splitter, C3 in PGP product

- The HYSYS Dynamic model (dotted) runs with plant data (solid) every minute.
- Second column: C3 in top (scale 0.2 to 0.3%) and other variables like floating pressures and flows are following the plant variations.
Case Study 6: Double C3Splitter, C3 in PGP product

- The HYSYS Dynamic model (dotted) runs with plant data (solid) every minute.
- First column SP of C3 in top changes from 0.34% to 0.37% (0.03% change!) and the inferential anticipate the analyzer response.
Your takeaways
Customer presentation about using HYSYS Dynamics to generate massive virtual plant data to develop ML soft-sensor

Send email to: josemaria.ferrer@inprocessgroup.com

Easy to read whitepaper about Best Practices to request and exploit Lifecycle Digital Twins

Visit our webpage, or

Excel file to tune the AspenIQR BIAS-update parameters (Tau1, Delay1, ABIASFRAC, etc)
Thank you!

Q&A

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