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

**independent** from any provider (process simulator or ICSS)

**our core business** is Process Simulation

keen to **share its knowledge** with clients

**Mission**
Help our clients to achieve **safer**, **greener**, **more reliable** and **more profitable** industrial operations

**Inprocess Solutions & Services**

**Lifecycle Modelling and Operator Training Simulators**

**Process Simulation Studies**

**Professional Development & Training**

**Applications and Software Products**

© Inprocess
Emissions Challenges in the Process Industry

Issues

- Tracking internal states that cannot be measured
- Sensor solutions prohibitively expensive
- Real-time tracking virtually impossible through measurements
- Dynamic operation
- Regulators limits

It is extremely valuable to know what is internally happening with the most critical components in the process
  - Even if we cannot measure them directly

Let's test solutions to the monitoring issue
We need a case study that allows us to benchmark a new solution for this problem
• That accounts with enough historical data
  • For normal operation AND abnormal operation
• Simple enough to handle so that we can get insights
• Complex enough so that it is representative of the process industry dynamics
• That does not compromise client’s data privacy

We select the Tennessee Eastman Process as our reference problem
Problem statement:
- Consider one of the components as a critical component
- The component is hard to track due to recycle and reactions

<table>
<thead>
<tr>
<th>Component</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>2.0</td>
</tr>
<tr>
<td>B</td>
<td>25.4</td>
</tr>
<tr>
<td>C</td>
<td>28.0</td>
</tr>
<tr>
<td>D</td>
<td>32.0</td>
</tr>
<tr>
<td>E</td>
<td>46.0</td>
</tr>
<tr>
<td>F</td>
<td>48.0</td>
</tr>
<tr>
<td>G</td>
<td>62.0</td>
</tr>
<tr>
<td>H</td>
<td>76.0</td>
</tr>
</tbody>
</table>

A + C + D → G
A + C + E → H
A + E → F
3D → 2F

Small losses through the product stream
Unavoidable losses
Problem statement:
- Consider one of the components as a critical component
- The component is hard to track due to recycle and reactions
- Let’s track the A inventory of this plant

<table>
<thead>
<tr>
<th>Component</th>
<th>Molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>2.0</td>
</tr>
<tr>
<td>B</td>
<td>25.4</td>
</tr>
<tr>
<td>C</td>
<td>28.0</td>
</tr>
<tr>
<td>D</td>
<td>32.0</td>
</tr>
<tr>
<td>E</td>
<td>46.0</td>
</tr>
<tr>
<td>F</td>
<td>48.0</td>
</tr>
<tr>
<td>G</td>
<td>62.0</td>
</tr>
<tr>
<td>H</td>
<td>76.0</td>
</tr>
</tbody>
</table>
How can we estimate our inventories and losses? (as accurately as possible)

1. Plant measurements
2. First-principles simulation
2. First-principles Simulation

- Dynamic replica of the asset, synchronized with real-time plant data.
- Tracking of the asset behavior
- Calculation of real-time values for temperature, pressure, flow, composition and inventories
2. First-principles Simulation

• Dynamic simulation provides valuable information of the trends and state of the plant
• But it has limitation in terms of accuracy and real-time trade-off

Can we improve first-principles estimation further taking advantage of historical data?
3. Data-driven Estimate Correction

Data-driven model

\[ \Delta^D y_t = \sum_{i=1}^{p} \phi_i \Delta^D y_{t-i} + \sum_{j=1}^{q} \theta_j \epsilon_{t-j} + \sum_{m=1}^{M} \beta_m X_m, t + \epsilon_t \]

\[ \epsilon_t \sim N(0, \sigma^2) \]

ARIMA Models

Online data

Offline data

Recurrent Neural Networks

General Form of RNNs

© by Inprocess
3. Data-driven Estimate Correction

Advantages of data-driven correction

- Can reflect differences between first principles and the actual plant that cannot be abstracted in the model
- Easy updating upon streams of new historical data
- Are only fed by variables measured in the plant and model
- Gives good results even for abnormal conditions
- The hybrid approach reduces the time-series dynamic load on the data-driven model
Inventory and emissions monitoring is becoming more important to address economic optimization and reduce greenhouse gas emissions.

Process simulation is one of the best tools in the market to understand and improve the behavior of your plant.

A data-driven layer on top of the simulation can provide a great way to target more specific goals for a digital twin and complement the model.
Iraola, E.\textsuperscript{1,2}, Nougués, J. M.\textsuperscript{1}, Batet, L.\textsuperscript{2}, Feliu, J. A.\textsuperscript{1} and Sedano, L.\textsuperscript{3}

\textsuperscript{1} Inprocess Technology & Consulting Group. Carrer de Pedro i Pons, 9. 08034 Barcelona
\textsuperscript{2} ETSEIB, Universitat Politècnica de Catalunya · BarcelonaTech (UPC), Department of Physics. Av. Diagonal 647, 08028. Barcelona
\textsuperscript{3} FUS_ALIANZ Science, Engineering & Consulting. Carrer Nord 19, àtic. 43700. El Vendrell

Eduardo Iraola, eduardo.iraola@inprocessgroup.com

www.inprocessgroup.com