Developing inferentials based on Digital Twins: Distillation case studies

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inprocess

Agenda

- Who we are
- I don´t want to believe: Analyzer vs. Peng-Robinson
- Our Lifecyle 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

independent from any provider (process simulator or ICSS)

our **core business** is Process Simulation

enthusiastic about **sharing its knowledge** with our clients

2006
est. in Barcelona by domain experts

55 countries
worldwide presence

60+
simulation engineers

380+
years experience

400+
executed projects

330+
training courses

Inprocess Solutions & Services

Lifecycle Modelling and Operator Training Simulators

Process Simulation Studies

Professional Development & Training

Applications and Software Products

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

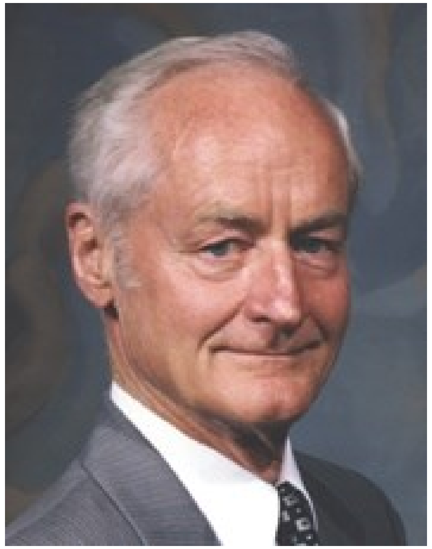
Strangely enough, plants are following those laws

Analyzers versus Peng-Robinson

How much do you trust in them?

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

We use them to control the plant



Ding-Yu **Peng** Don **Robinson**

University of Alberta, Department of Chemical and Petroleum Engineering

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

We use them to design the plant

Our Lifecyle Digital Twin vision

Also called:

LifeCycle Operator Training Simulator (LC OTS)

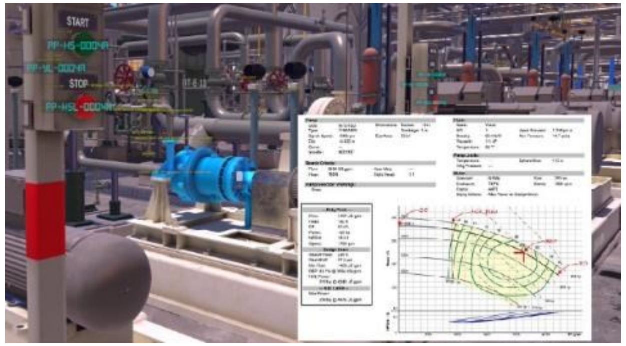
Or

Multi-Purpose Dynamic Simulator (MPDS)

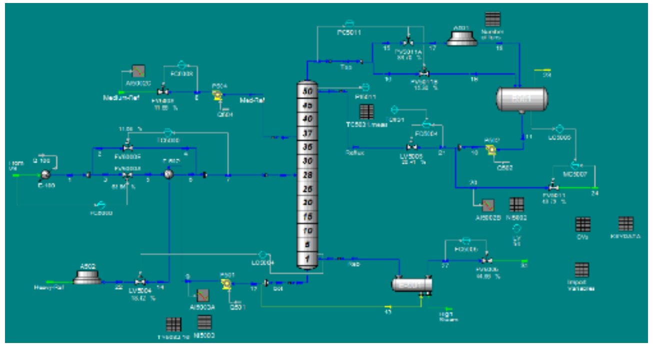
Inprocess' Approach to Digital Twins

- **Digital Twins are virtual copies of physical assets and their operating behaviours**
- **This definition has several points of view which are complementary to each:**

Contextualized 3D models

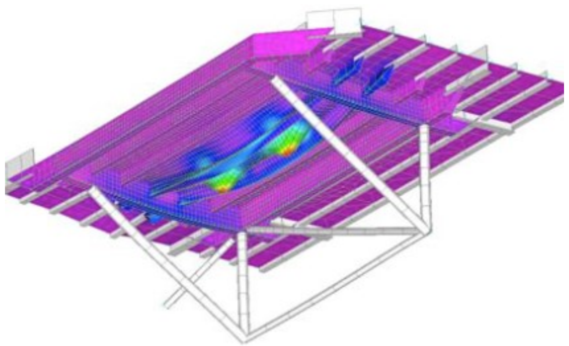


First-Principles Models

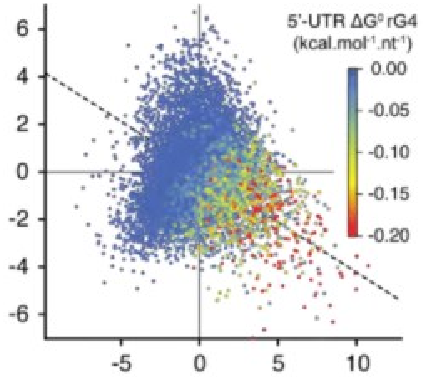


Digital Twins

Mechanical and structure models



Empirical Models (data fitting)



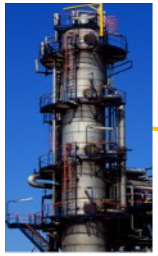
Centuries of Physics, Chemistry and Thermodynamics knowledge are consolidated here!

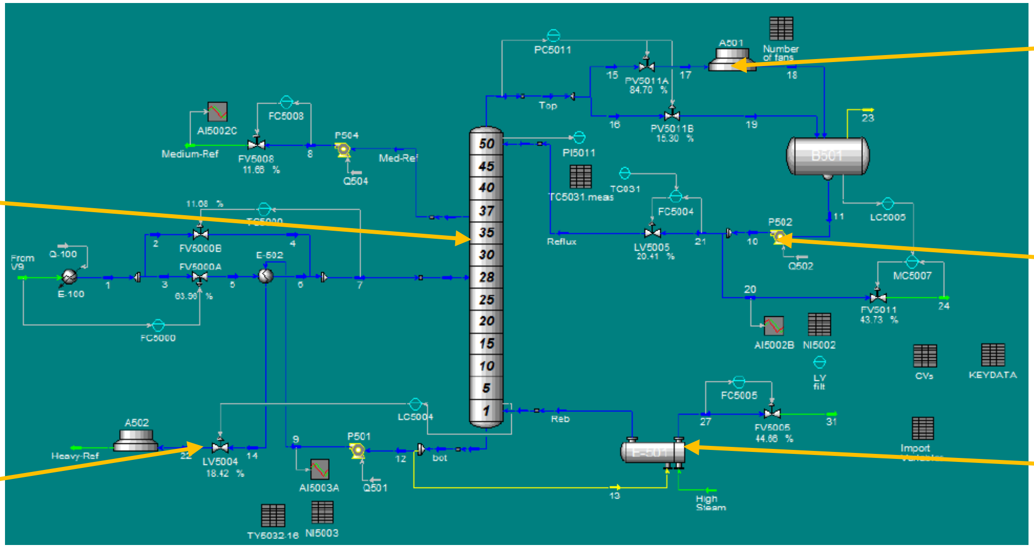
The Process Digital Twin concept

- **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).

Process Simulation Model
+
Inprocess Infrastructure Suite (IIS)
=
Inprocess' Digital Twin

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

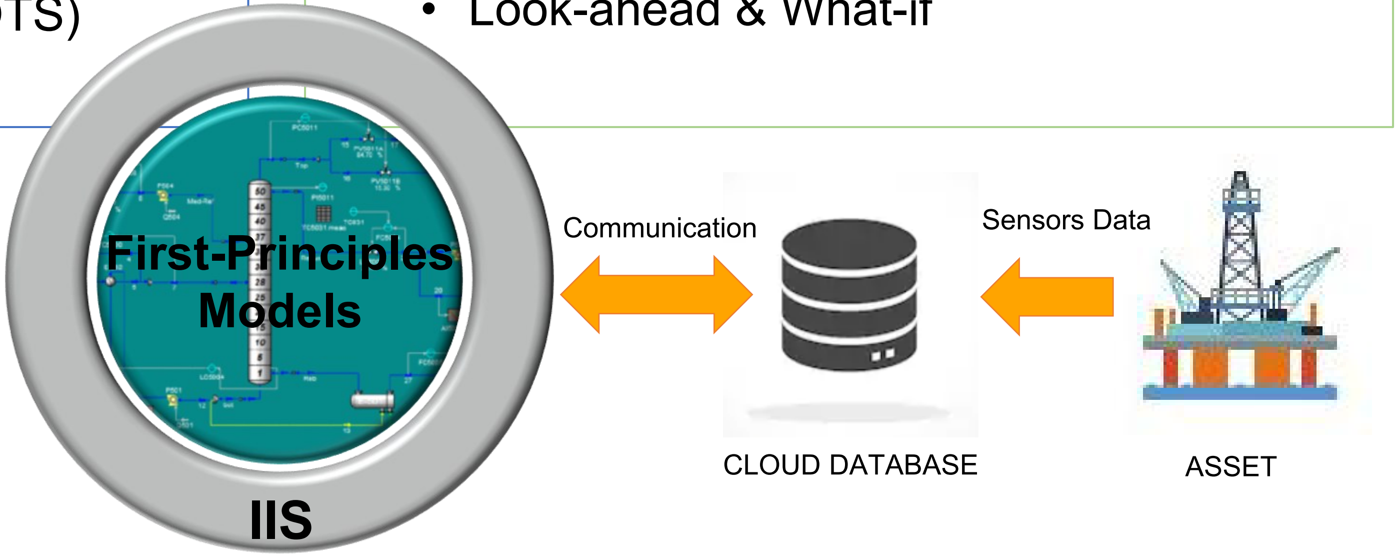
4 Operation-associated decision support and optimization

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



Developing Inferentials with Digital Twins

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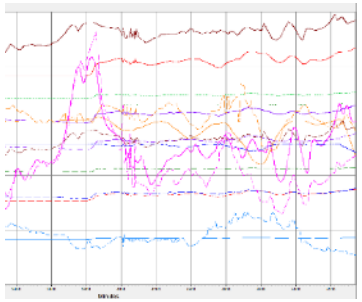
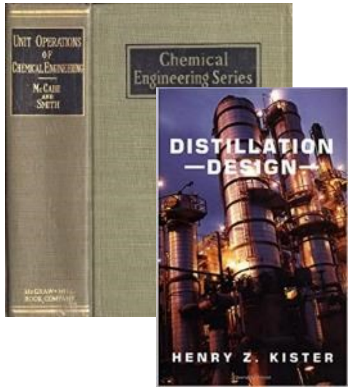
Finding the Truth with Industrial HI (Human Intelligence)



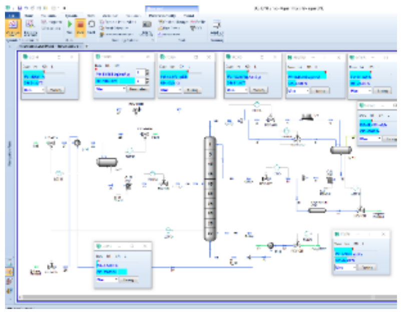
The Process Data

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

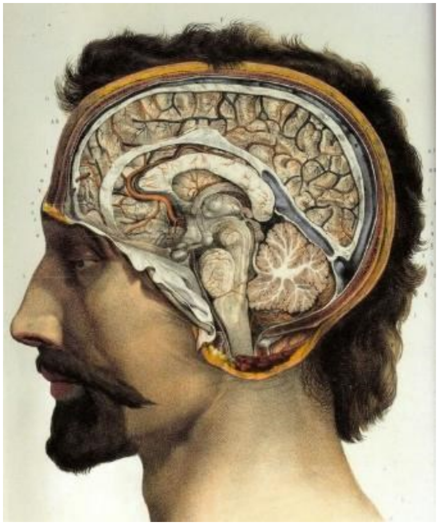
Hundreds of “Data Scientists” worked hard along the centuries to discover the laws of how matter behaves. Those **laws still last today**.



The Calculator

Process simulation is only a macro-compilation 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

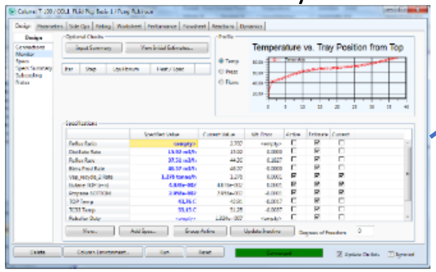
NO ↓

Dynamic effects? — NO → Column HYSYS Steady-State

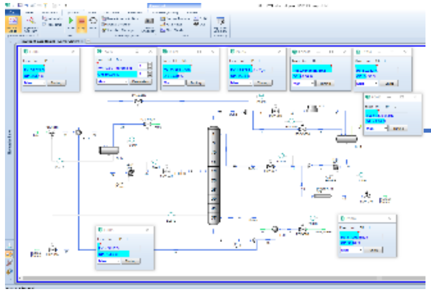
YES → Column HYSYS Dynamics

Simple HYSYS Steady-State

Column HYSYS Steady-State

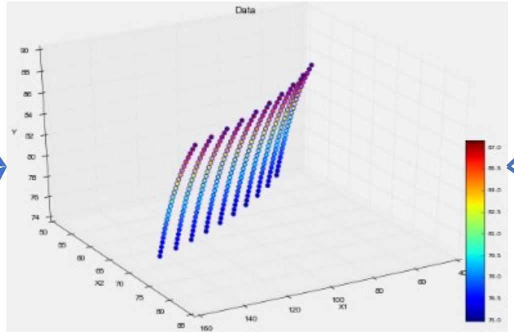


Column HYSYS Dynamics



Case Study

Case Study



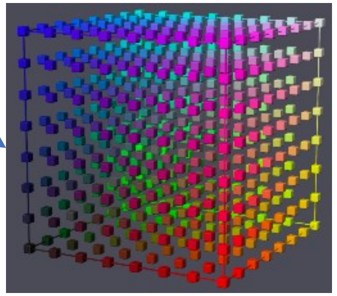
Feasible regression

No Feasible regression

Explicit Algebraic Formula for AspenIQ or DCS calc.

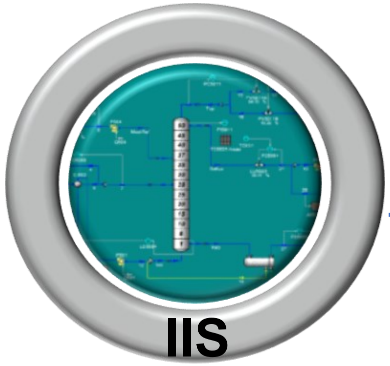
Example Formula= a + b*V1 + c*V2 + d*V1^2 + e*V2^2 + f*V1*V2	
a =	-124.125
b =	-1.7447543
c =	7.8426775
d =	-0.00104104771
e =	-0.06703829112
f =	0.02494089626
Correlation Coeff. (r):0.9971	

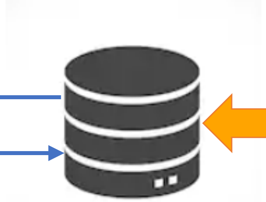
Online IIS lookup table

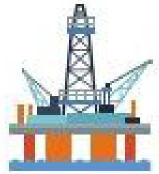


Configure IIS app and deploy

Online IIS + HYSYS Dynamics







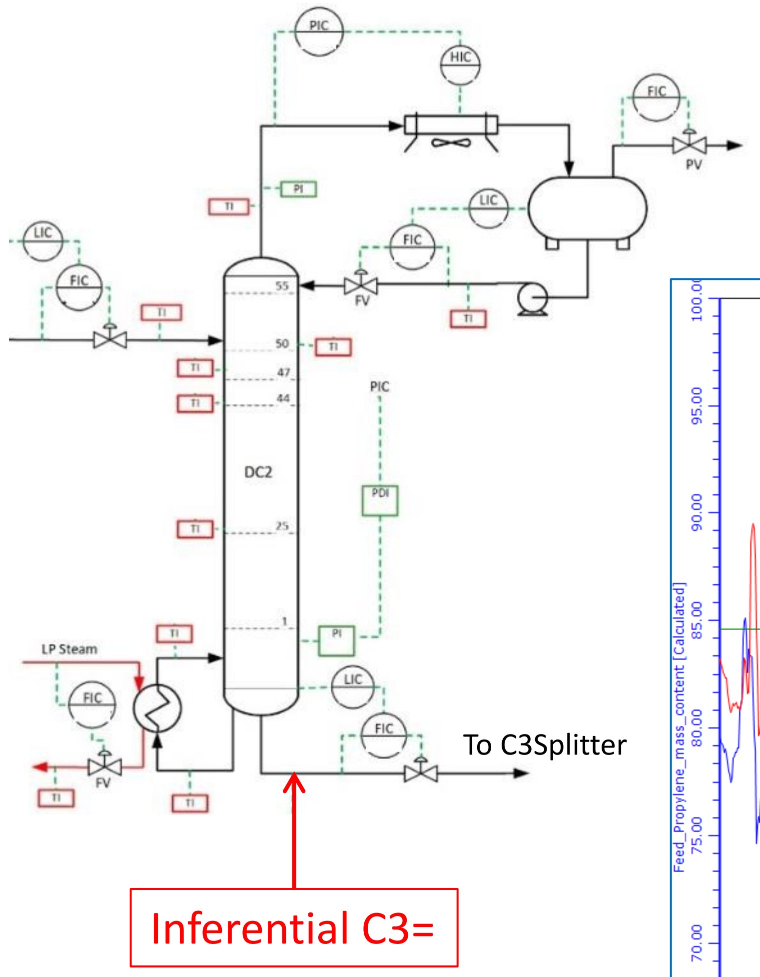
Customer RTDB:
Aspen IP21, OSI PI, CDF

Building distillation Inferentials with HYSYS

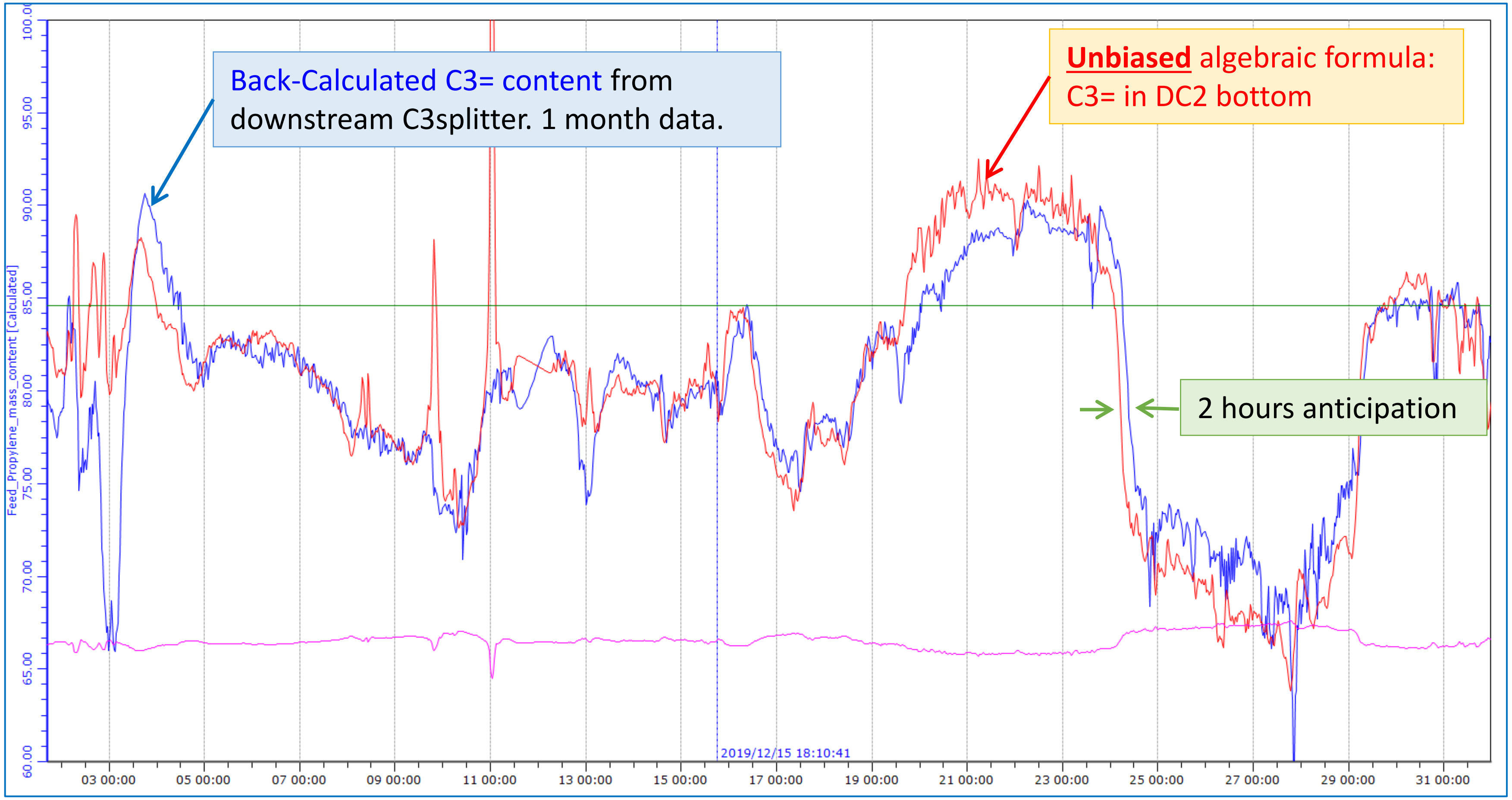
HYSYS case	Method	Deliverable	Time
Simple HYSYS case	Develop Multi-case study and correlation	Report with Explicit Algebraic Formula	2-3 days
Calibrated column with HYSYS Steady-State	Develop Multi-case study and correlation	Report with Explicit Algebraic Formula	2-3 weeks
	Develop Multi-case study, generate raw data set and install application	Online IIS application with Lookup table or HYSYS Steady-State	3-4 weeks
Calibrated column with HYSYS Dynamic	Configure and install application	Online IIS application with HYSYS Dynamics runtime	4 weeks (model from OTS) or 8 weeks

Customer Case Studies in distillation

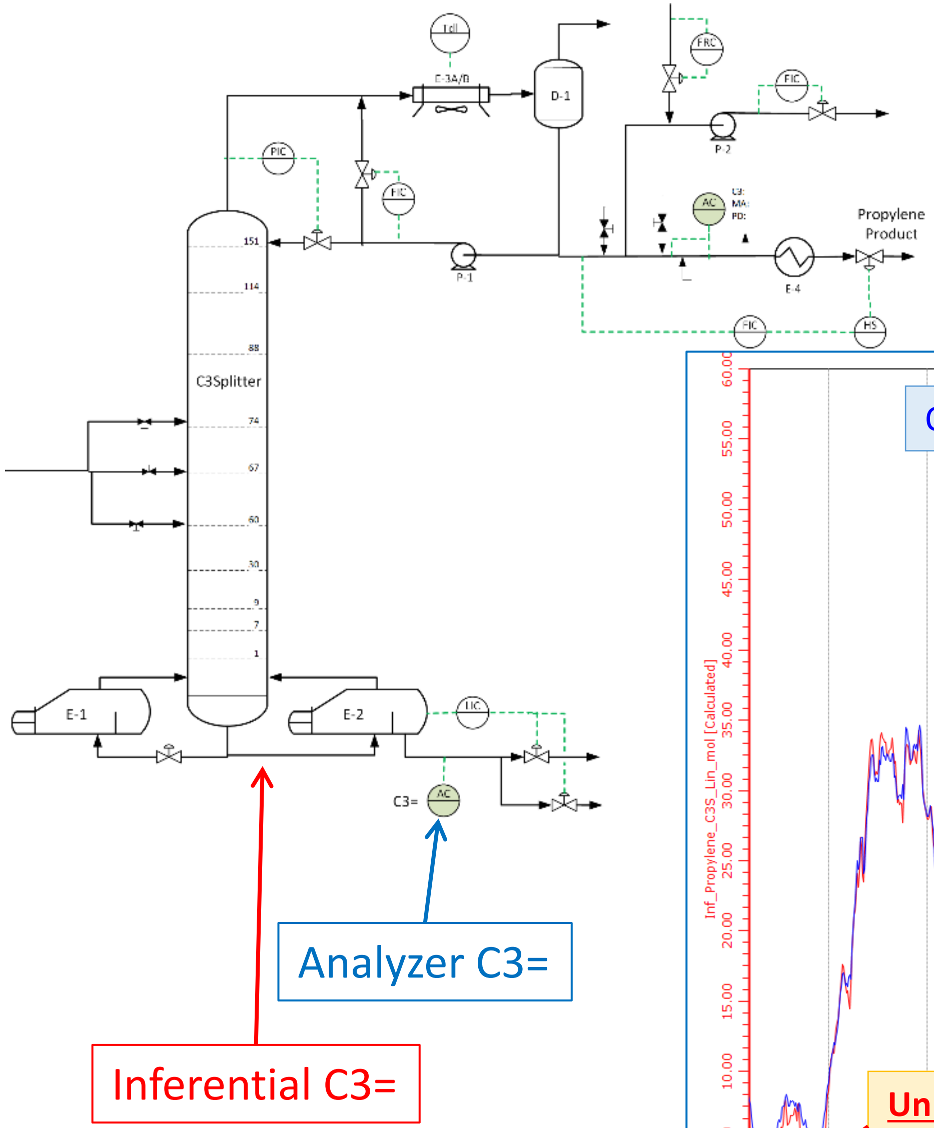
Case Study 1: C3= in Deethanizer bottoms



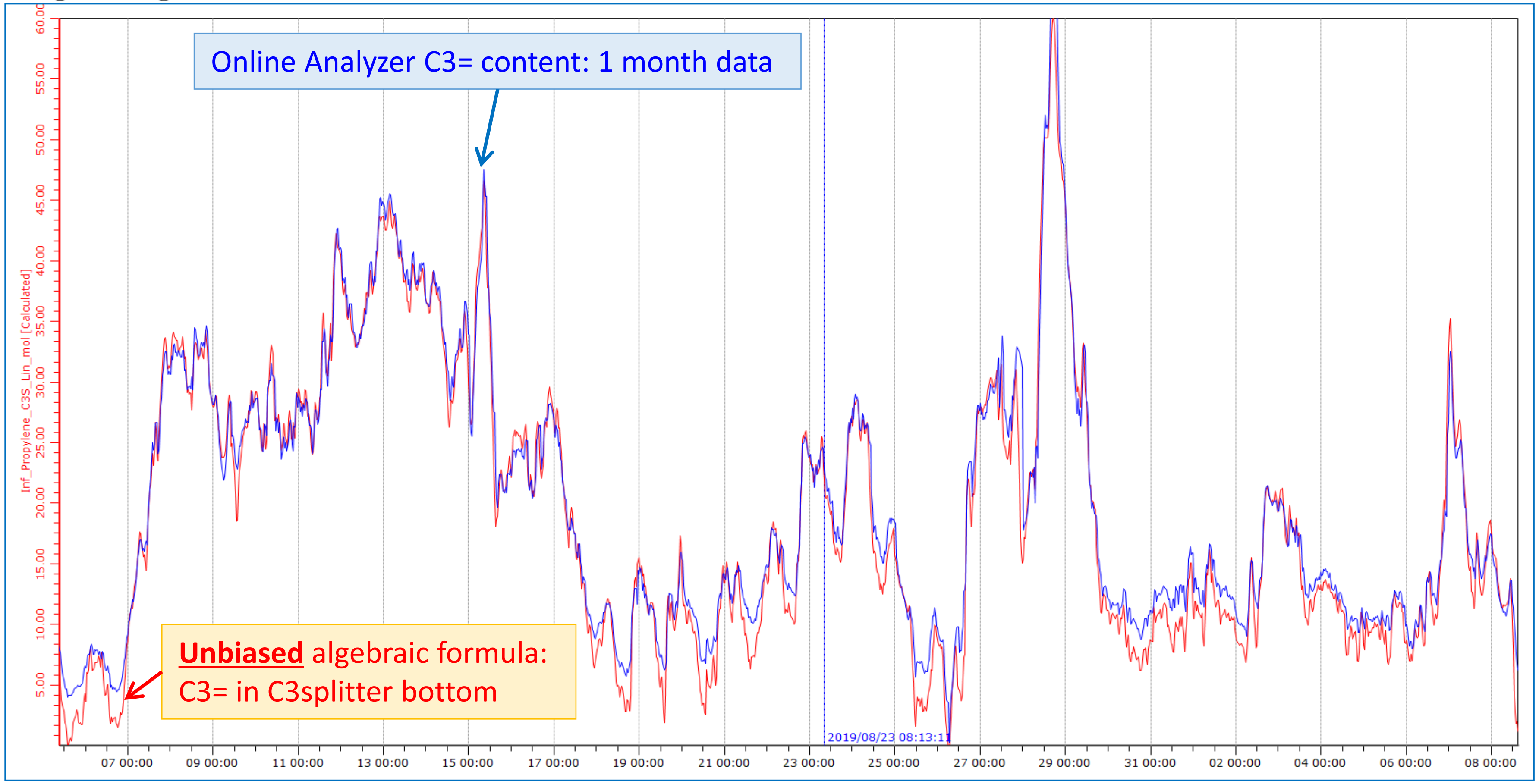
- For the APC controller of the downstream C3= Splitter it is important to infer the C3= content since it is an important FeedForward variable.
- Such an inferential can be calculated based on the Deethanizer bottoms conditions.
- HYSYS data was regressed to build an **Explicit Algebraic Formula**



Case Study 2: C3= in C3Splitter bottoms

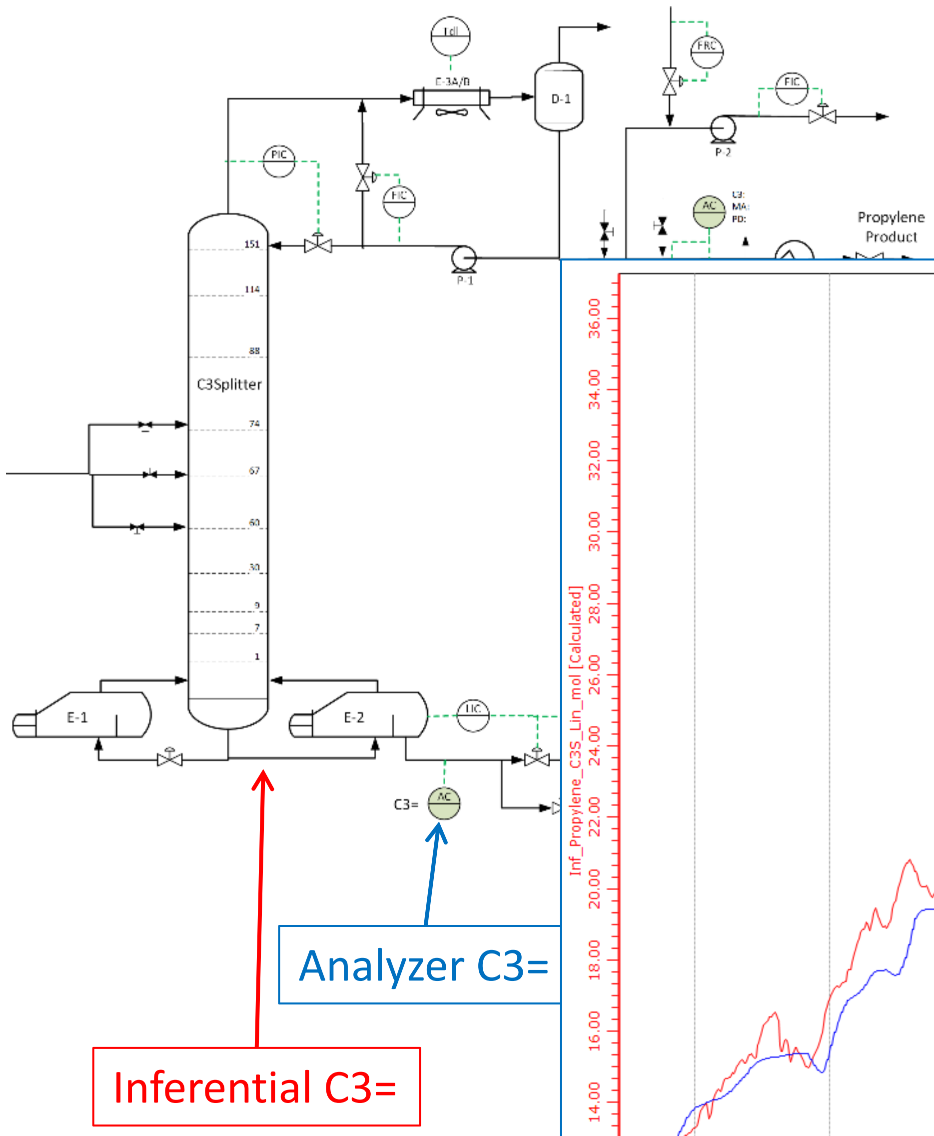


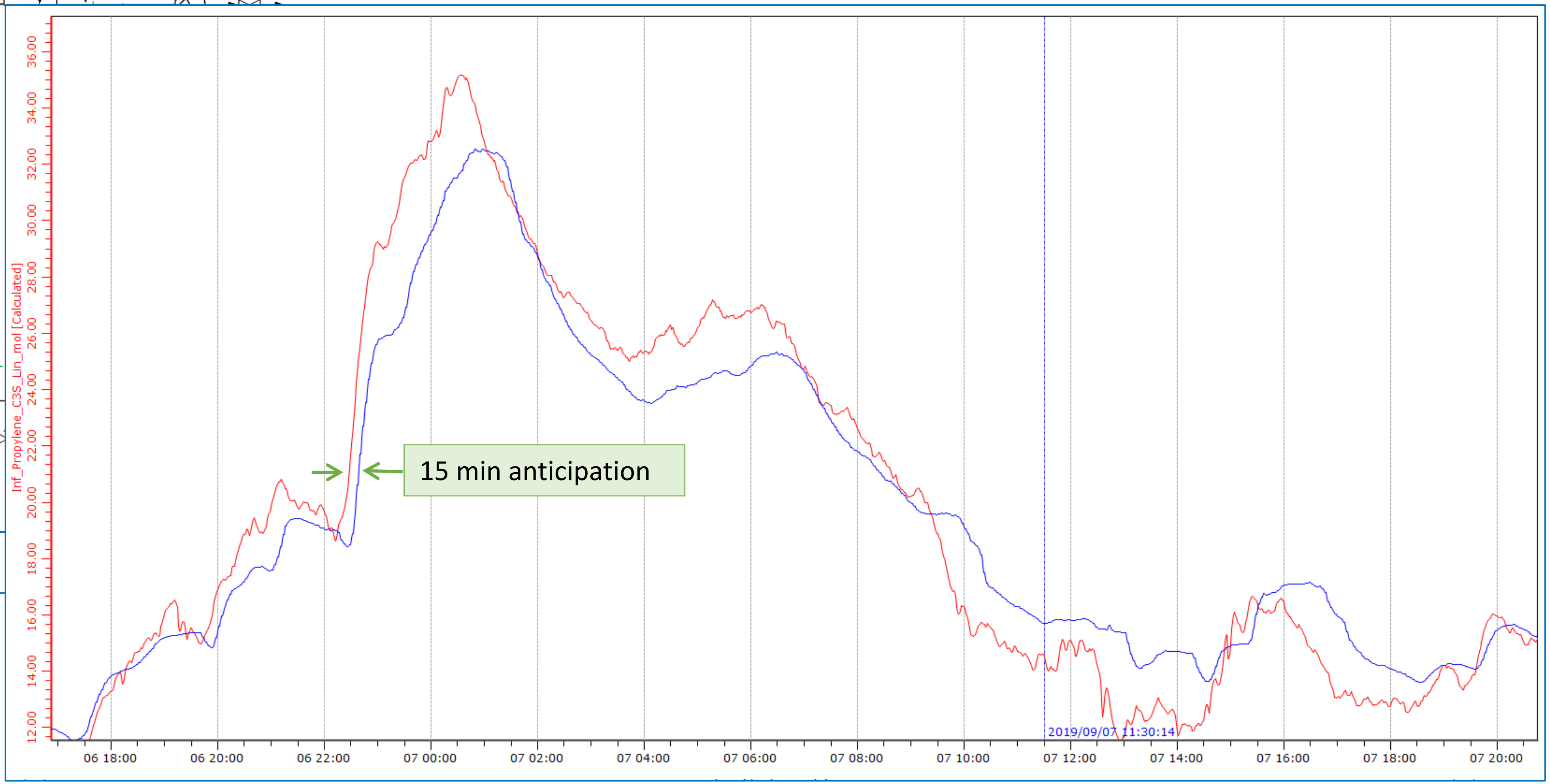
- C3= content in C3splitter bottoms is measured by Online Analyzer every 15 min.
- An inferential can provide a value every minute without the Analyzer delay.
- HYSYS data was regressed to build an **Explicit Algebraic Formula** for the inferential



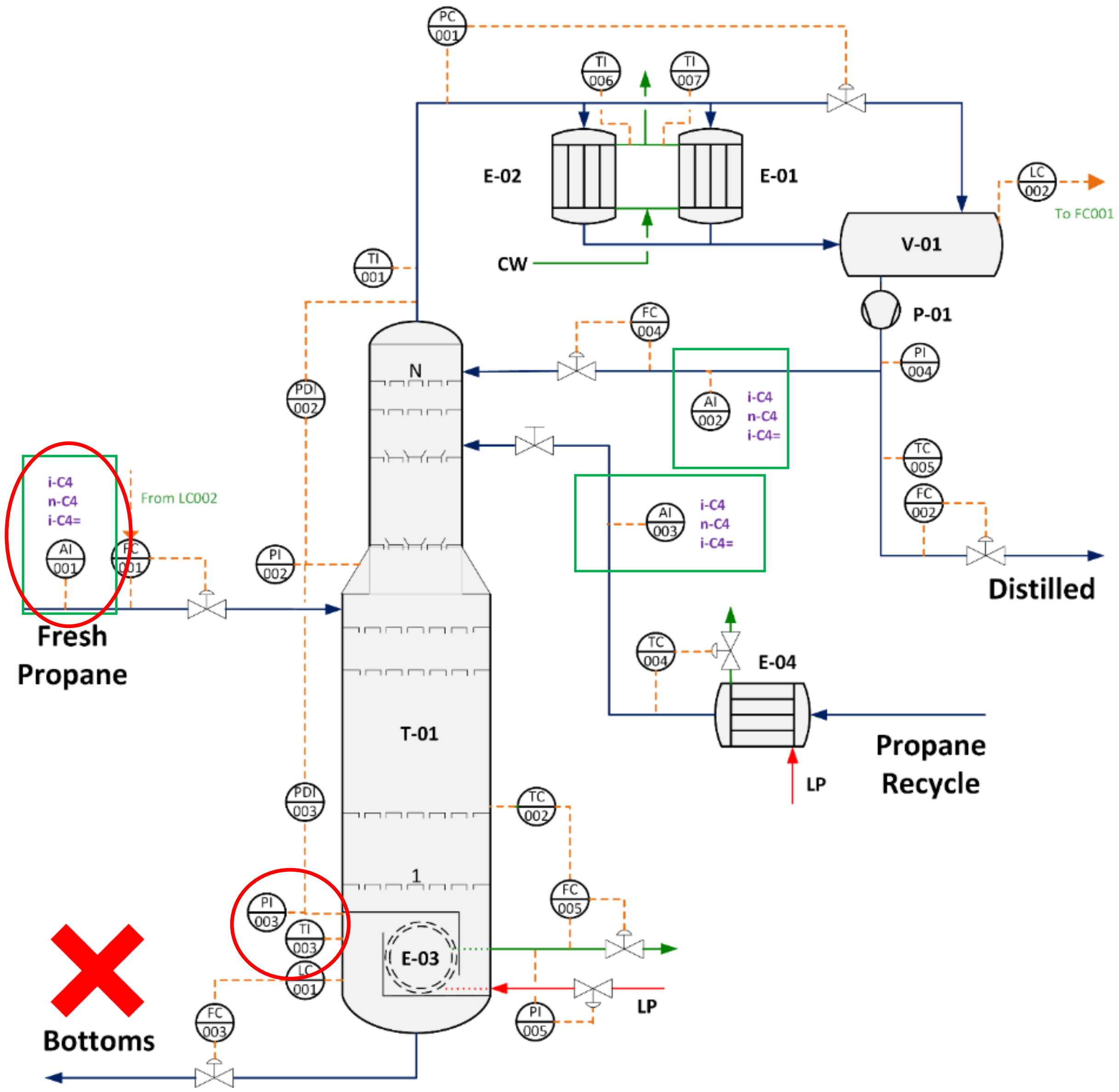
Case Study 2: C3= in C3Splitter bottoms

- 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

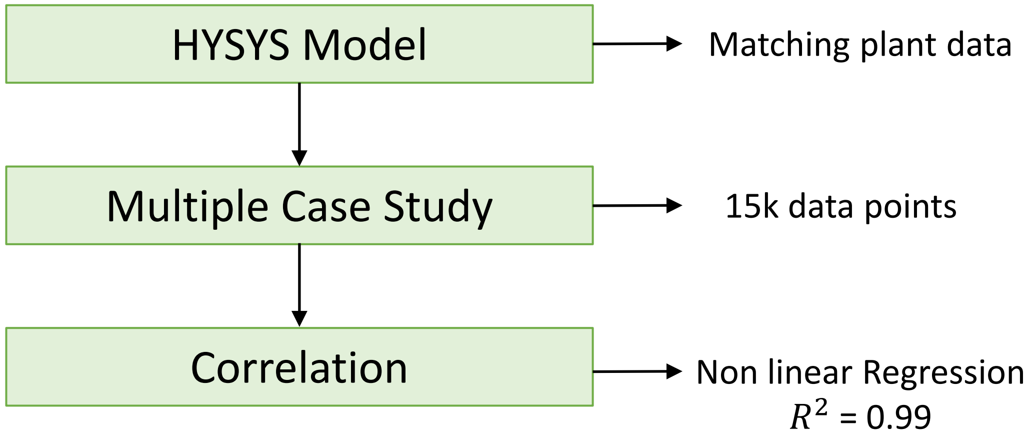




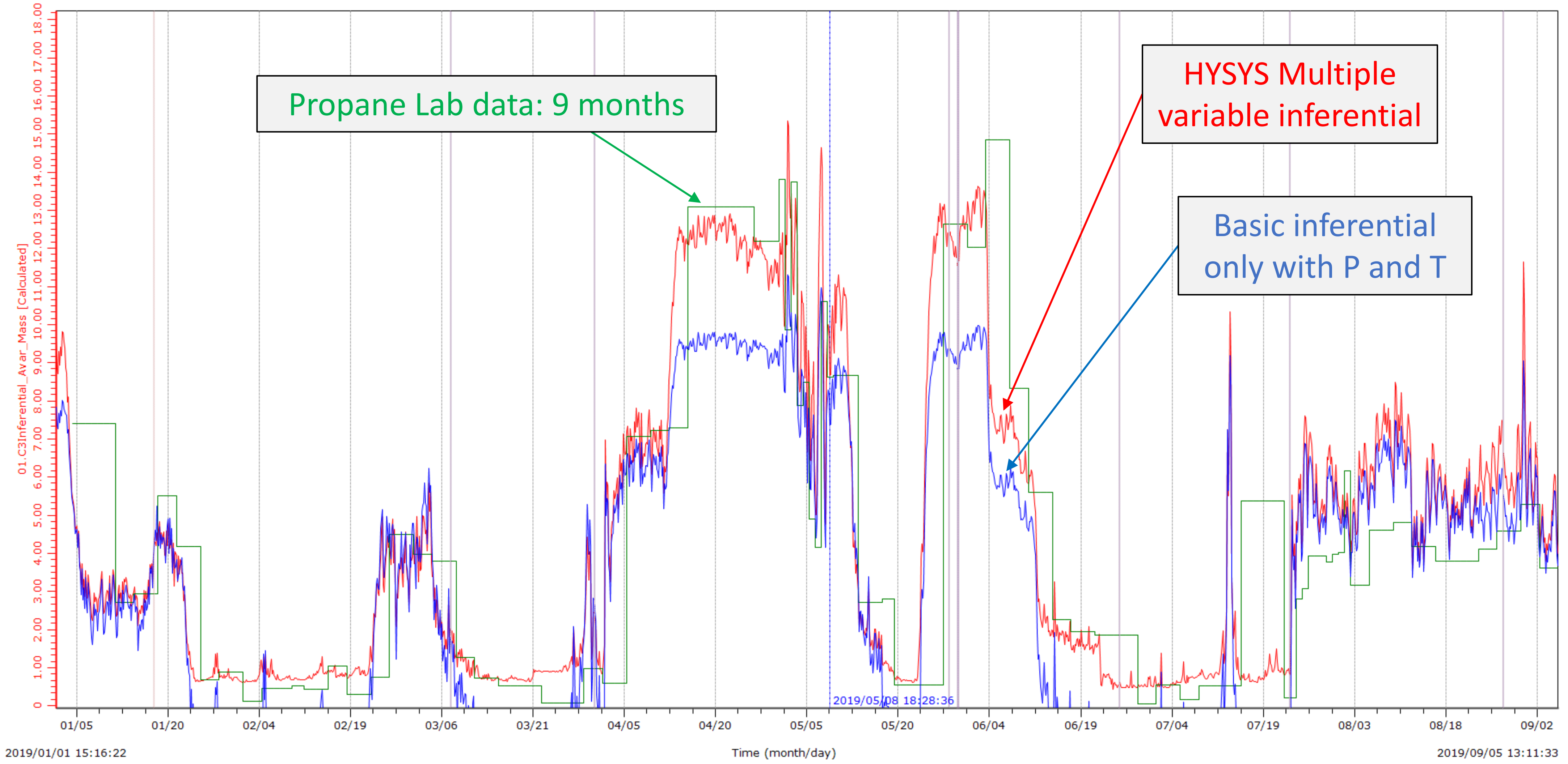
Case Study 3: Depropanizer bottoms



- 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**.

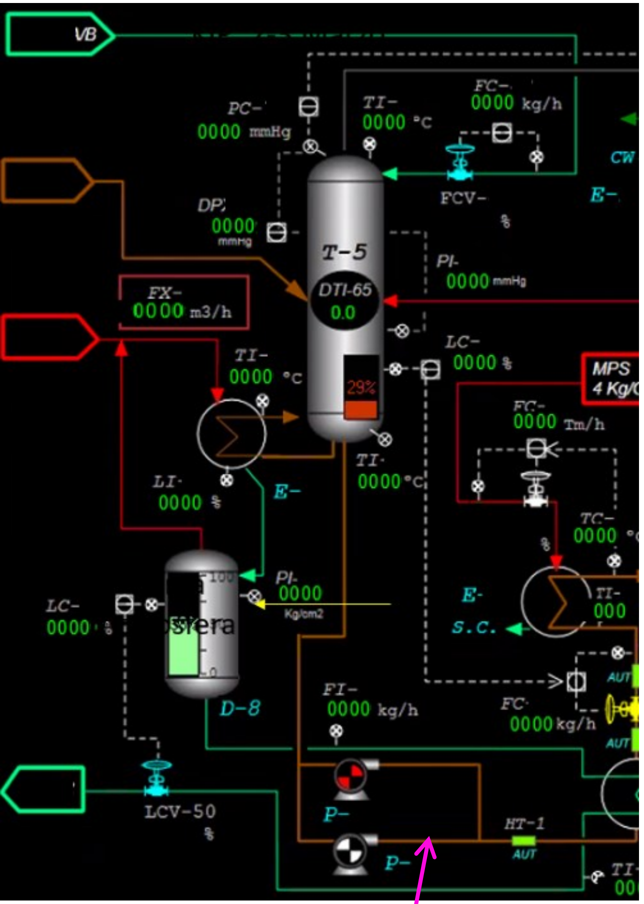


Case Study 3: Depropanizer bottoms

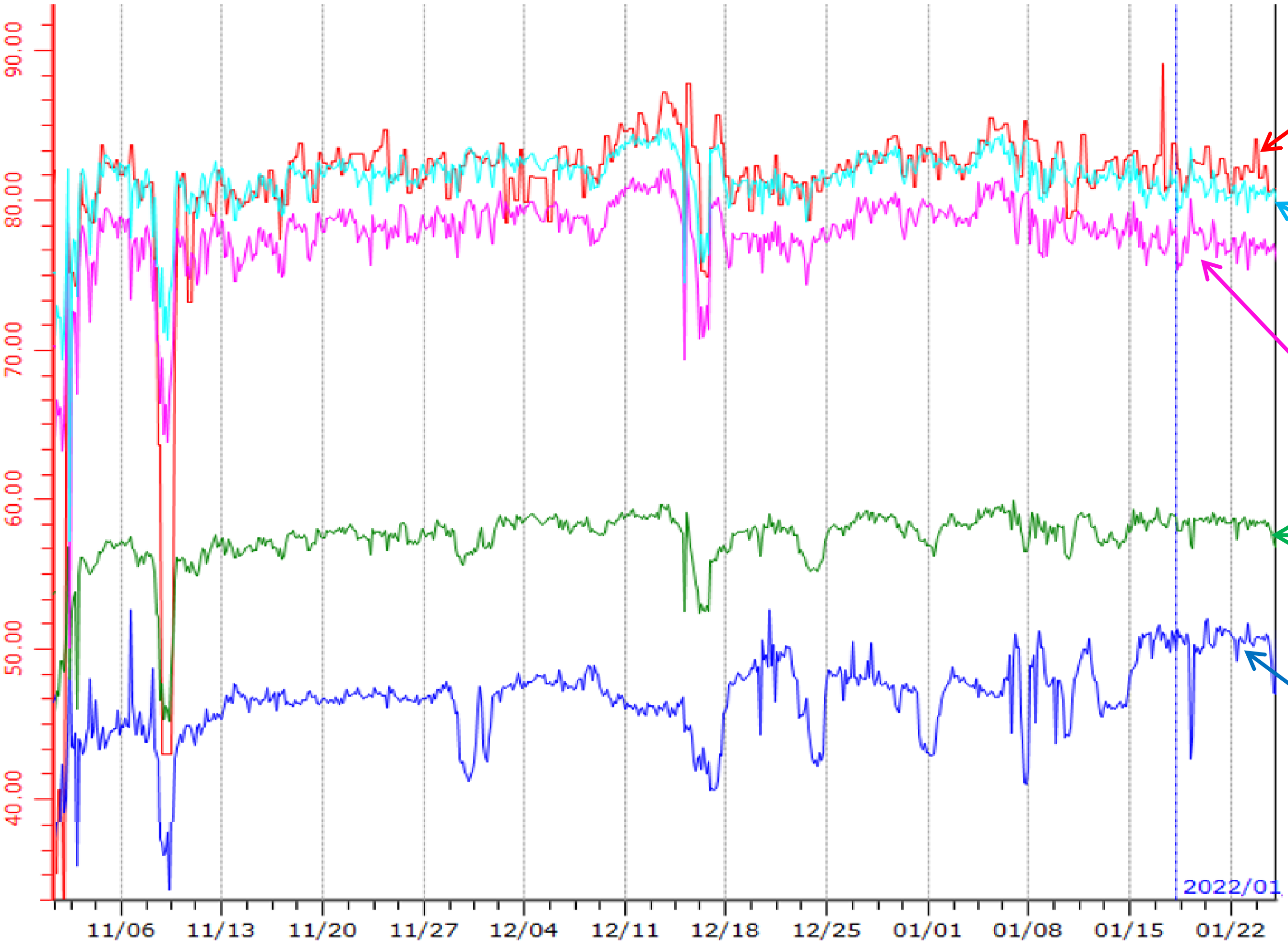


The graphic shows the unbiased inferential (just explicit formula without lab bias update)

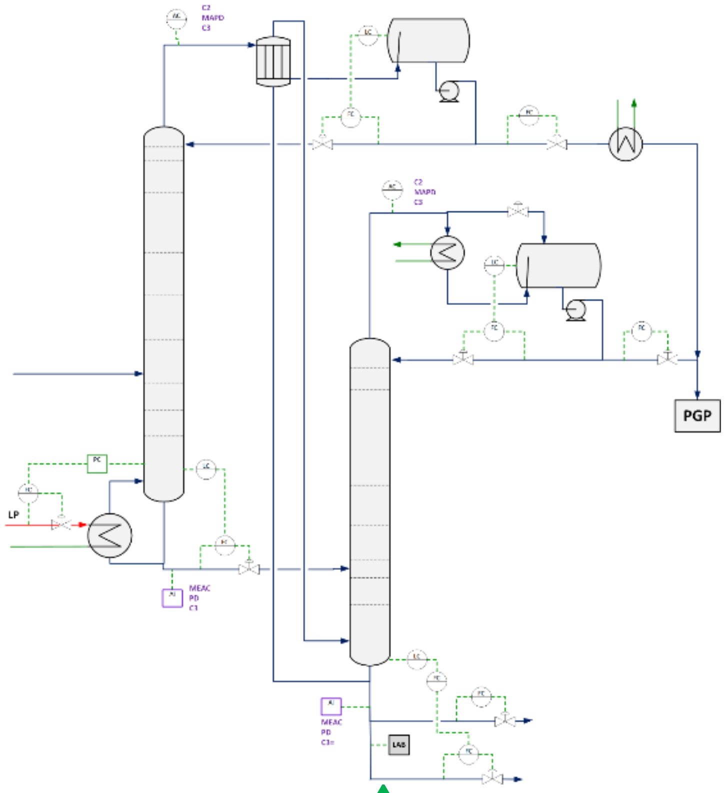
Case Study 4: Caprolactam in vacuum column bottoms



- Caprolactam content in column is sampled for LAB every 8 hours
- HYSYS data was regressed to build an **Explicit Algebraic Formula**



Case Study 5: Double C3Splitter, C3= in bottom



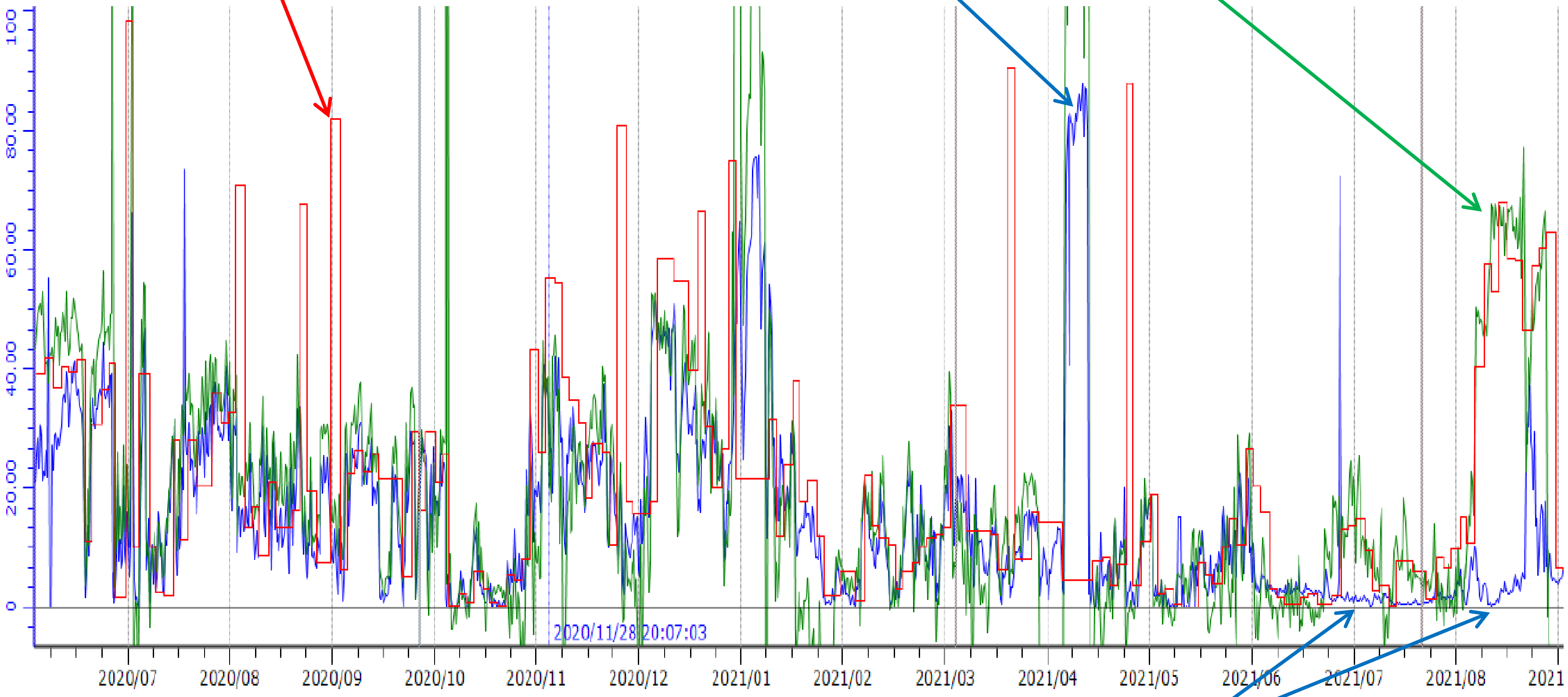
Inferential C3=

- 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.

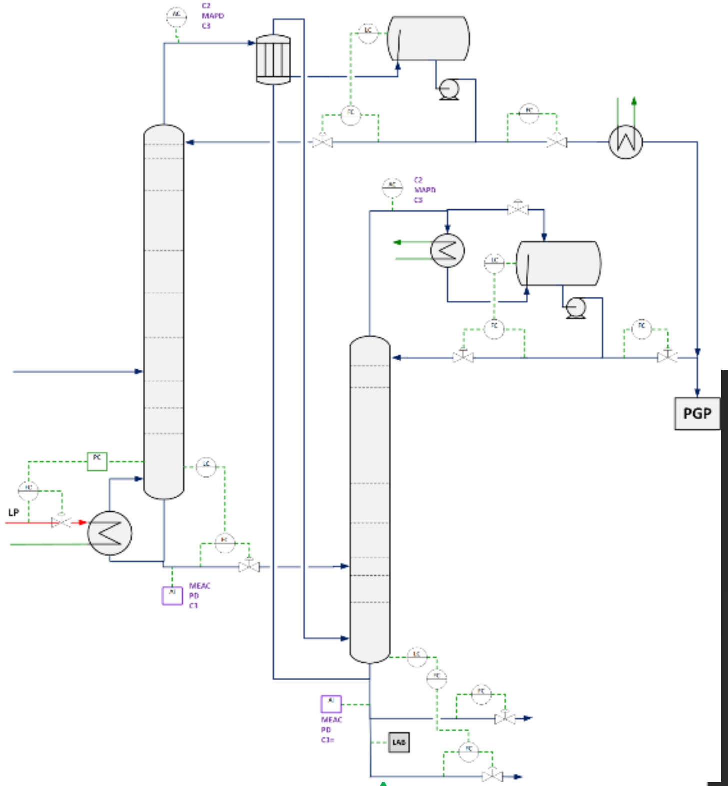
Online Analyzer C3= content

Unbiased algebraic formula: C3= in C3Splitter bottom



Online Analyzer DESCALIBRATION

Case Study 5: Double C3Splitter, C3= in bottom

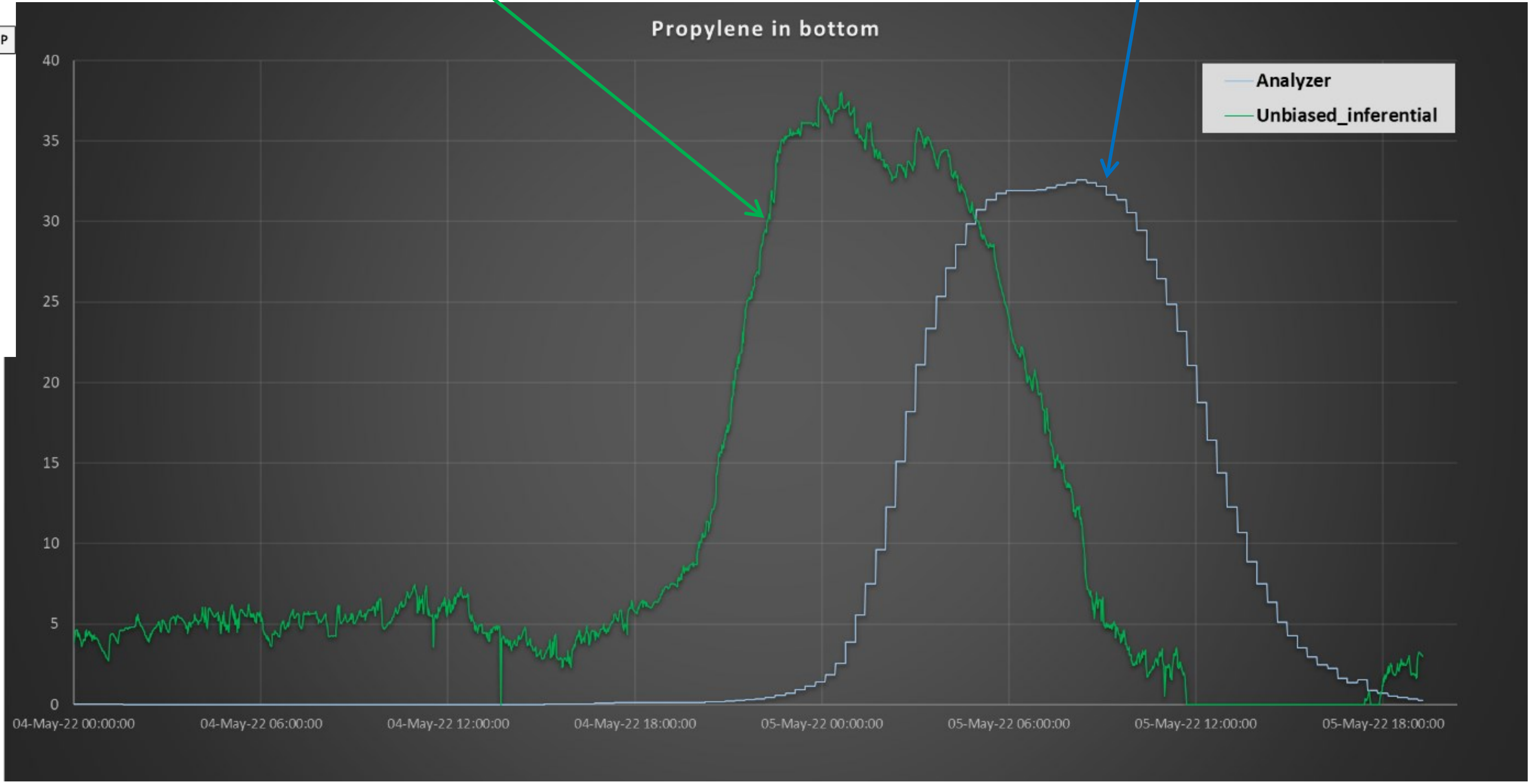


Inferential C3=

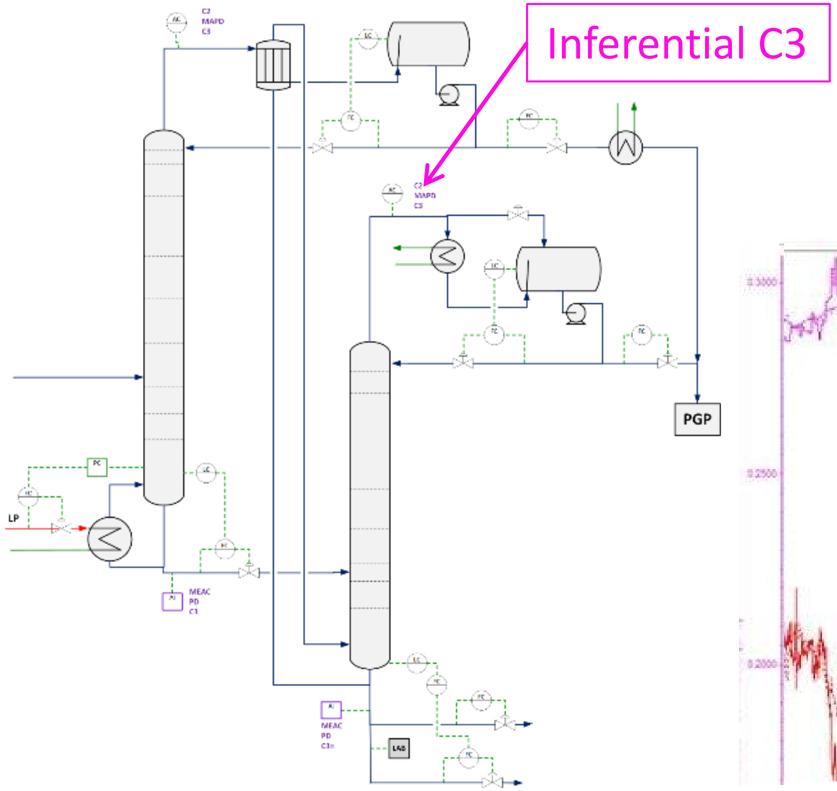
- The quality inferential was evaluated with a plant perturbation test. The inferential gave a 5 hour anticipation over the Online Analyzer.
- The Online Analyzer gives a false zero value out of the test.

Unbiased algebraic formula: C3= in C3Splitter bottom

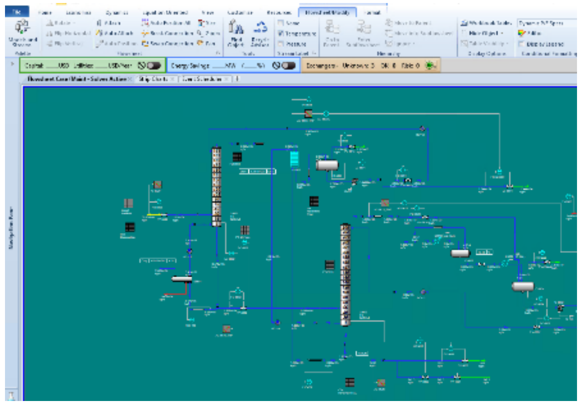
Online Analyzer C3= content

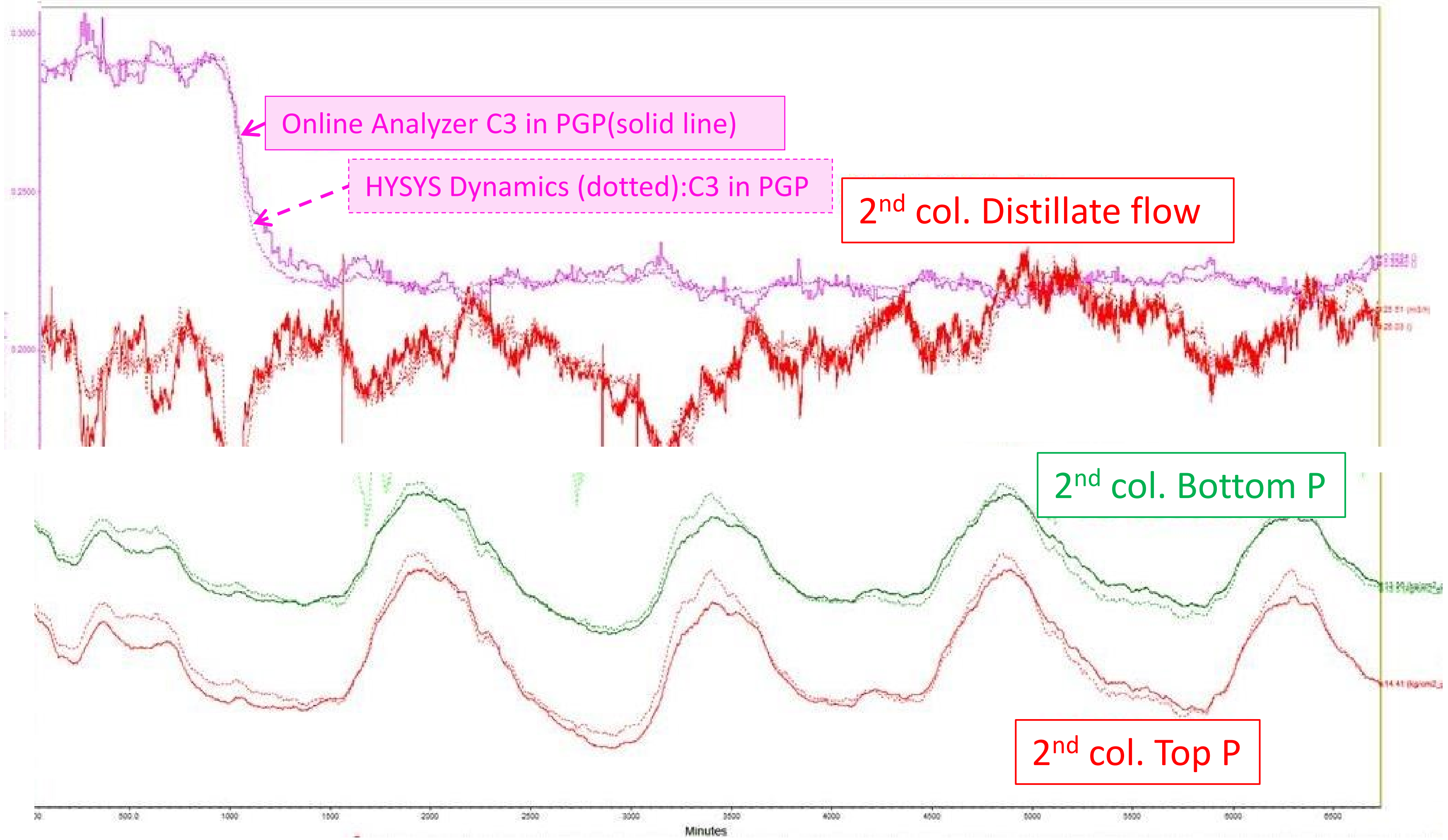


Case Study 6: Double C3Splitter, C3 in PGP product



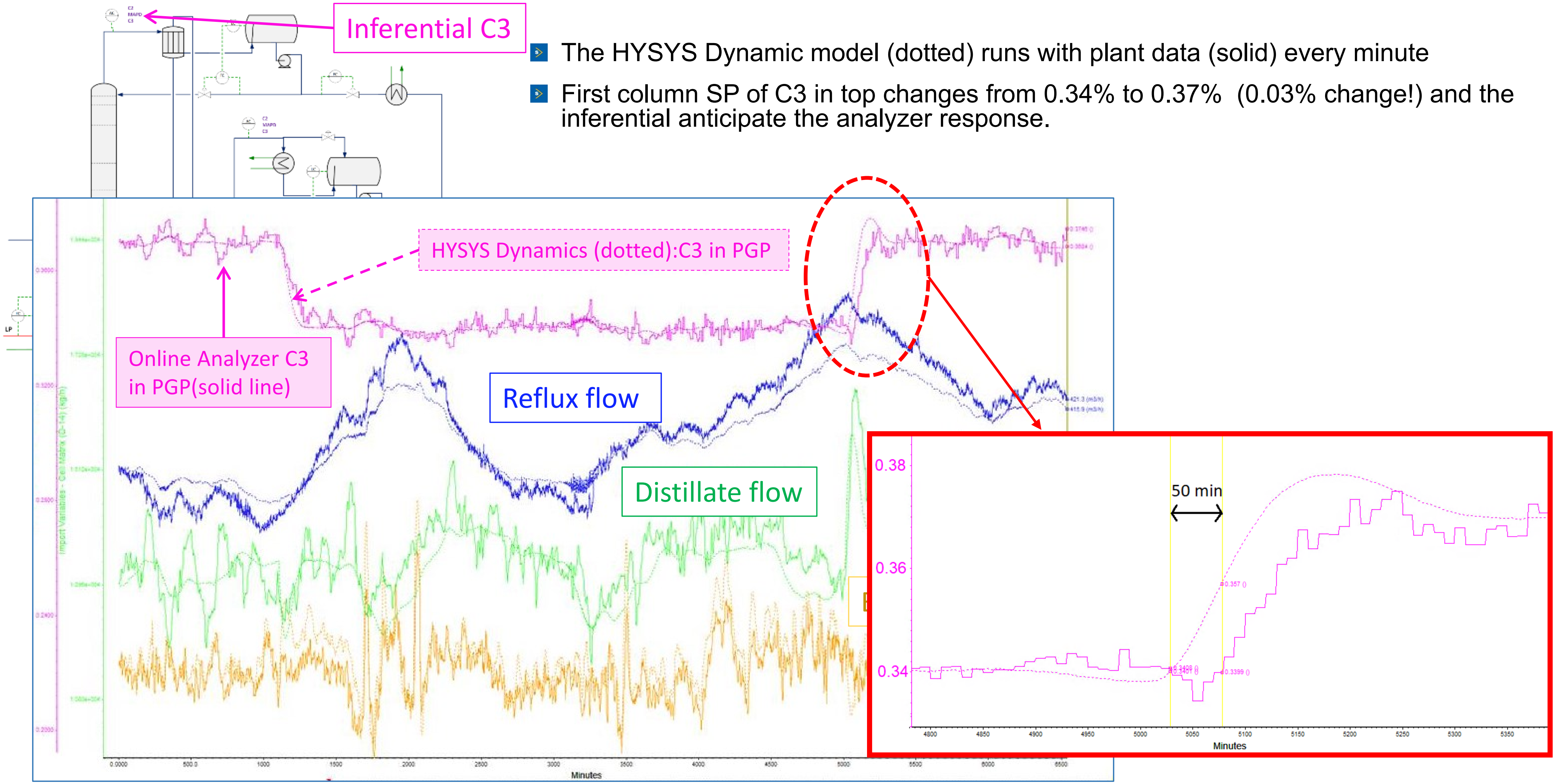
- The HYSYS Dynamic model (dotted) runs with plant data (solid) every minute
- Second column: C3 in top (scale 0.2 to 0.3%) and other variables like floating Pressures and flows are following the plant variations





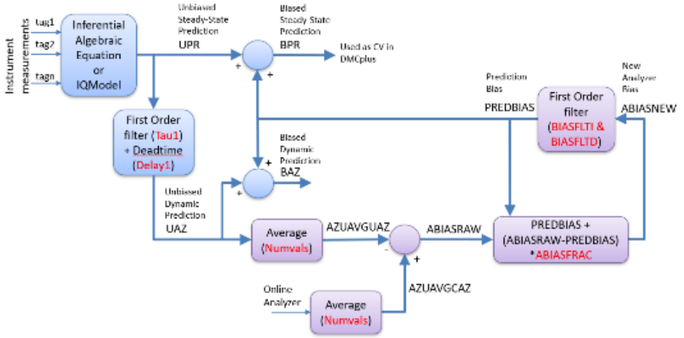
Case Study 6: Double C3Splitter, C3 in PGP product

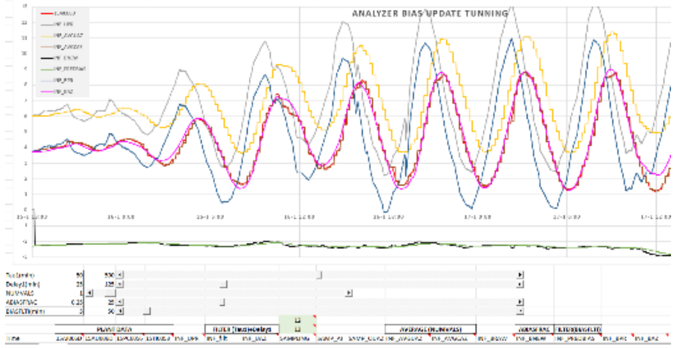
- The HYSYS Dynamic model (dotted) runs with plant data (solid) every minute
- First column SP of C3 in top changes from 0.34% to 0.37% (0.03% change!) and the inferential anticipate the analyzer response.



Your takeaways

Your takeaways





Excel file to tune the AspenIQ BIAS-update parameters (Tau1, Delay1, ABIASFRAC, etc)

Send email to:
josemaria.ferrer@inprocessgroup.com

Customer presentation about using HYSYS Dynamics to generate massive virtual plant data to develop ML soft-sensor

Visit our webpage, or Google

CEPSA softsensor HYSYS

1

Break free

Every OpCo, EPC and Licensor has their own process simulation preferences. Many man-hours and other resources have been invested in learning this specific software, in developing the process models and even in creating internal property packages or custom unit operations.

Consequently, if a company has standardized the usage of a specific simulation software (e.g. Aspen HYSYS), it should be able to request/demand an OTS using the same simulation engine and not be limited to the process simulation tools offered by the ICSS vendors.

Frequently, ICSS vendors tend to install the Main Automation Contractor (MAC) schemes in new projects and constrain the customers to acquire the OTS exclusively from them, without giving any option to the EPC or OpCo to freely decide what process simulation software they prefer to use in their OTS.

By decoupling the OTS from the MAC, or by specifying your preferred process simulation software, you are securing the quality of the most important component of the OTS: The Simulation Engine. Therefore, you are selecting the process simulation software based on best standards rather than a low-fidelity

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

Visit our webpage, or Google

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Thank you!

Q&A

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JoséMaría Ferrer

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