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# Online Simulations: Challenges and Opportunities for Process Performance Monitoring

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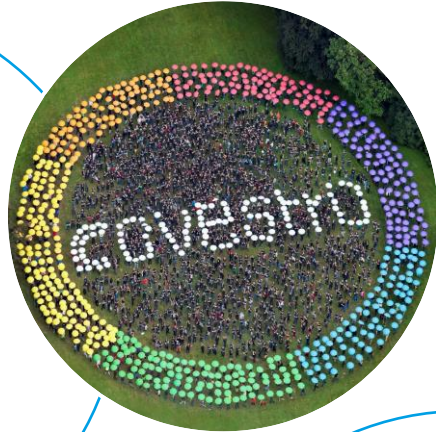
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# Covestro – leading in the world of plastics



## Strong

- €10.7 bn in sales
- 16,500 employees<sup>1</sup>



## Useful

- Plastics, precursors and solutions
- For many industries



## Global

- 50+ production sites globally
- Close to customers and partners



## Innovative

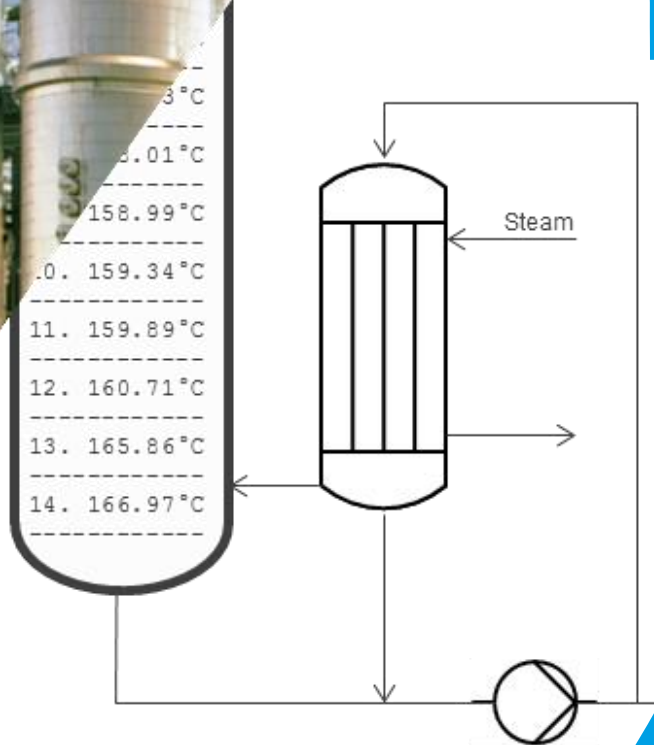
- 1,200+ employees in research and development
- 80 years of ideas and inventions





# Challenges and Opportunities for Online Simulations for Process Performance Monitoring

Maria Sofia Palagonia,  
Christian Bratfisch,  
Kristian Voelskow



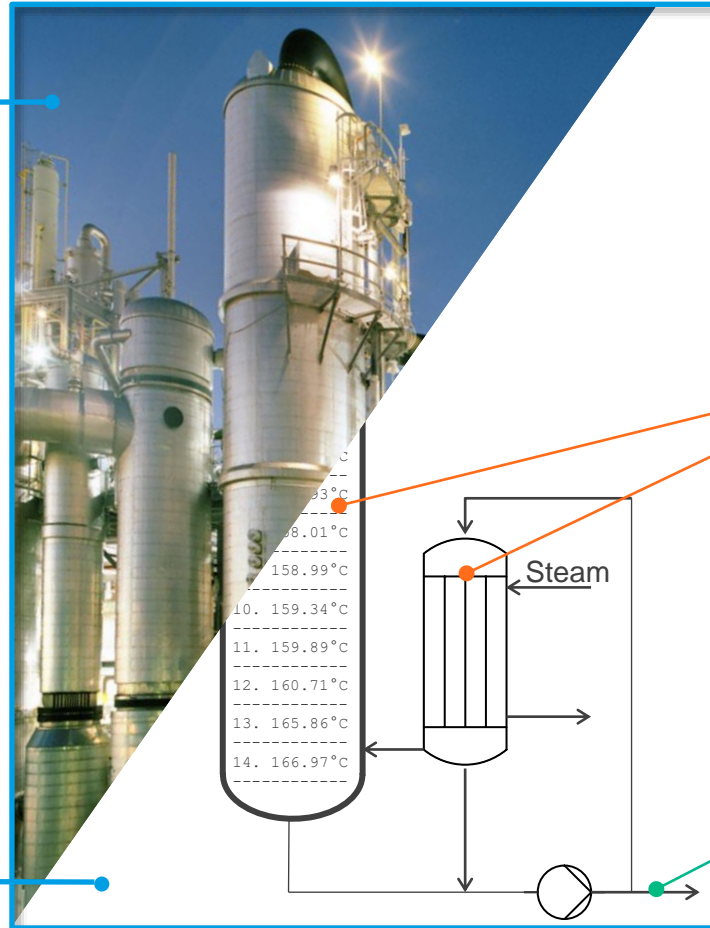
# Online Simulation: Overview



Process with live measurements



Mass & energy balance model



Energy Demand

Get direct conclusion on minimum steam consumption

Fouling

Anticipate cleaning intervals for heat-exchanger & column

Product purity

Monitor the amount of undesired side-components

# Outline

## Two use cases of Online Simulation

## Technical Insights

## Further developments

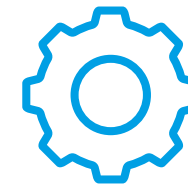
Which process insight do we calculate from our models and which benefits do we extrapolate?



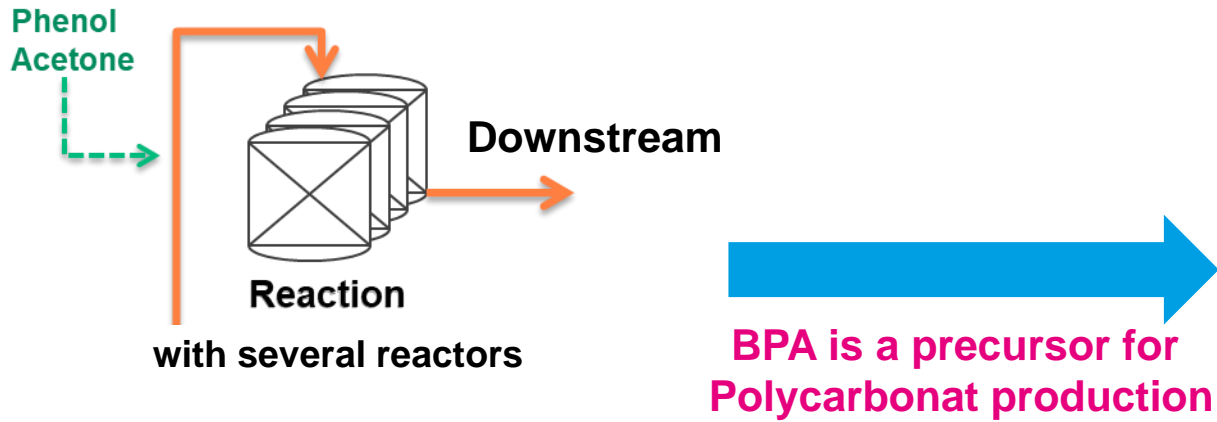
How we improve capabilities thanks to PI-AF and APS



Infrastructure: from in-house servers to the cloud



# Model for BPA Reactor



## Sample applications



For automotive  
applications



For modern  
notebooks



For lifesaving  
medical devices



Infrastructure for  
5G transmission  
technology

# Online Model for optimized catalyst exchange scheduling

## Goal:

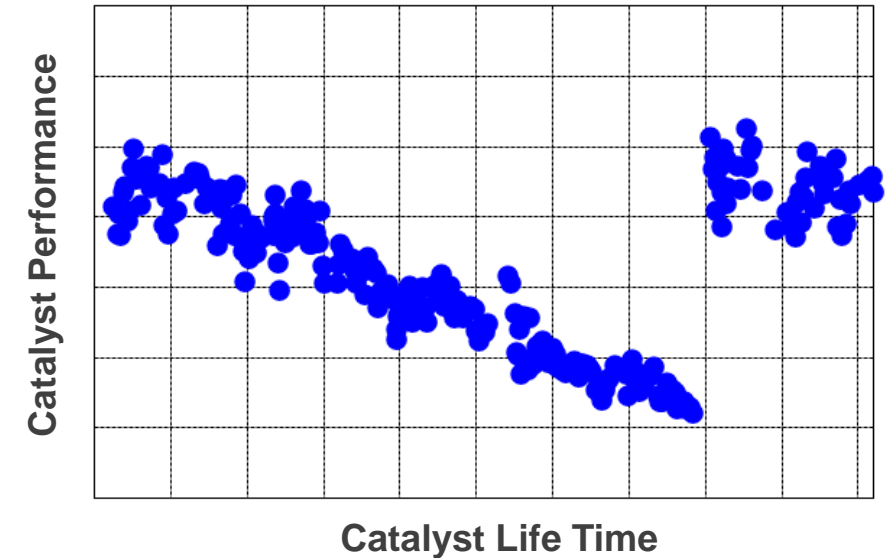
- Monitoring of catalyst deactivation
- Based on model data prediction of future catalyst demand

## Potentials:

- Ensure maximum BPA production
- Efficient planning of upcoming catalyst exchanges

## Challenges:

- Steady state: process fluctuations create significant uncertainty in model evaluation
- Broken transmitters

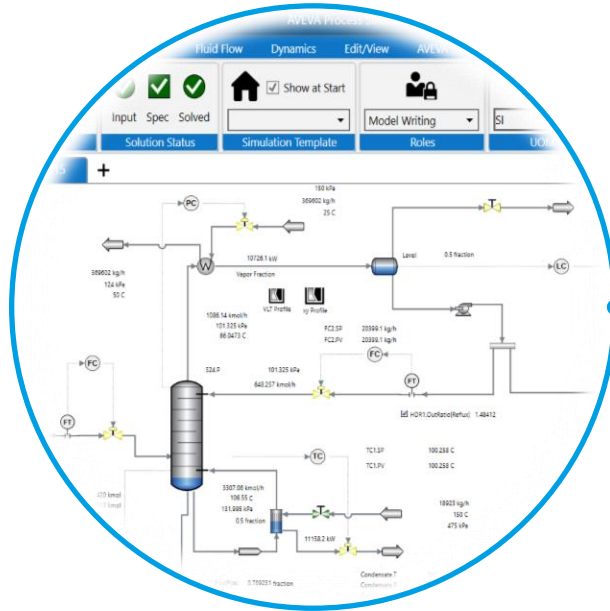




# New Opportunity – Aveva Process Simulation

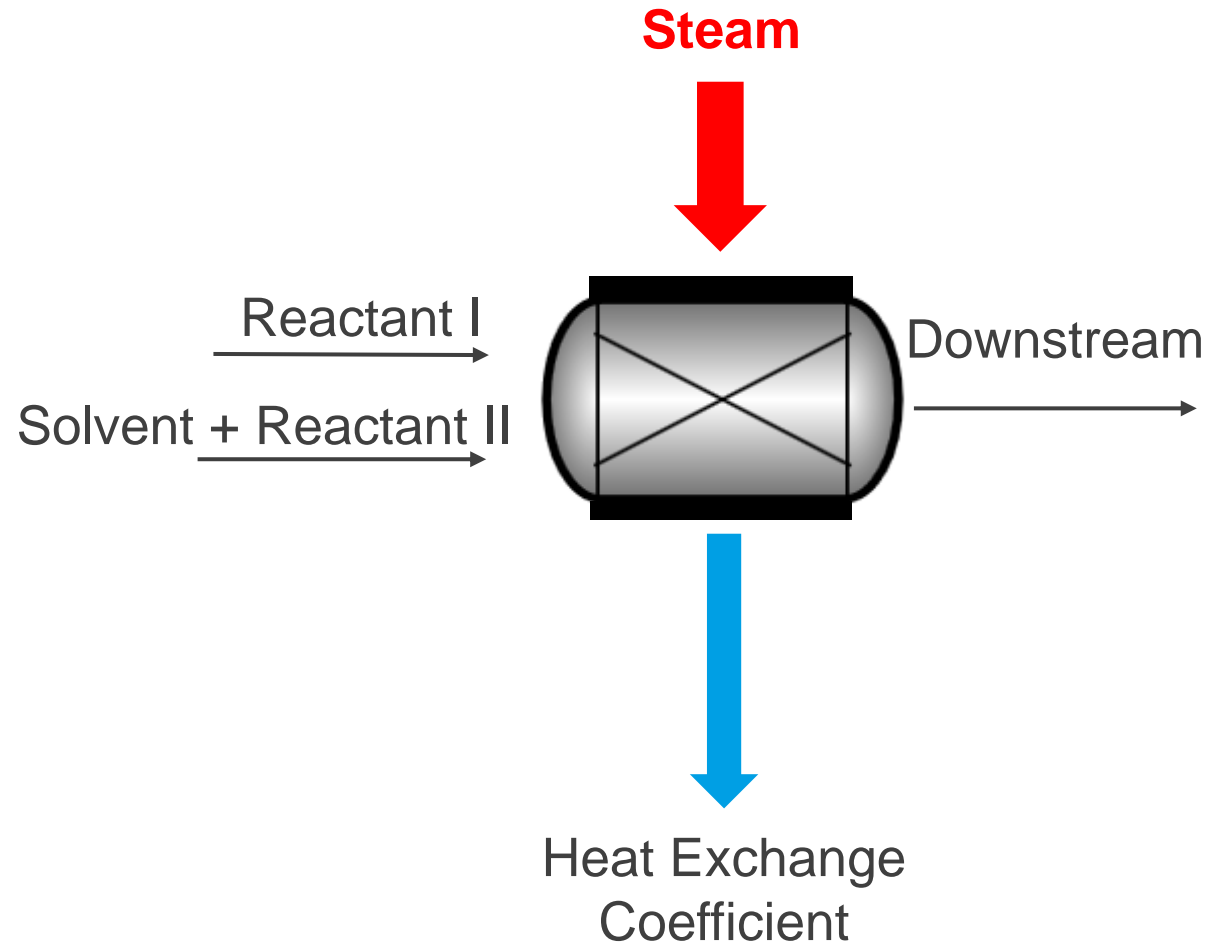
## Aveva Process Simulation

- Graphical user interface
- Python interface to control model
- Plenty additional features

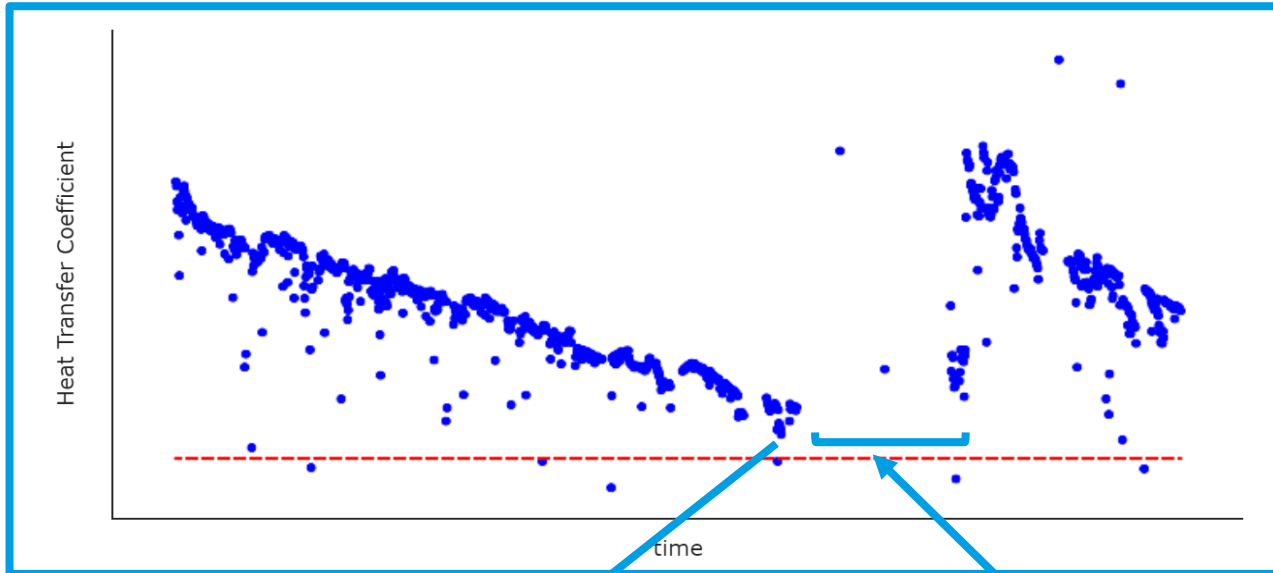


Applied use case:  
Monitoring of  
reactor fouling to  
plan the next  
cleaning

# What is my model calculating?



# Which is the key value from the model results?



Next  
cleaning  
activity!

## Goal:

- Monitoring of reactor fouling to ensure efficient heat exchange

## Potentials:

- Timely planning of upcoming cleaning activity

# Share & Connect

## Navigate

Select the asset

## Monitoring KPIs

Fouling,  
concentrations,  
energy demand, ...

## Optimization

Get operational  
recommendation

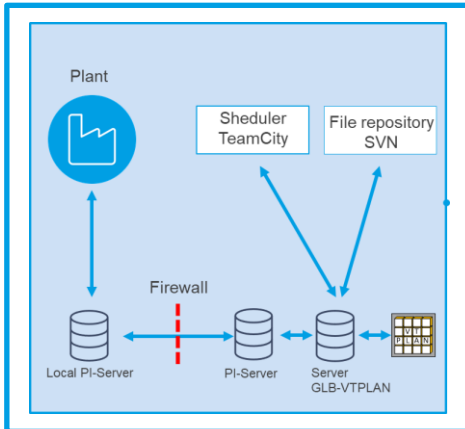


→ KPIs can directly be accessed by plant operation

# Challenges

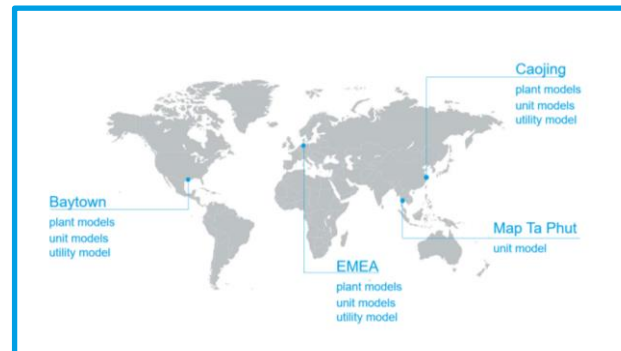
## Architecture

- Must be extensible and scalable, but also flexible and maintainable
- Model/data management



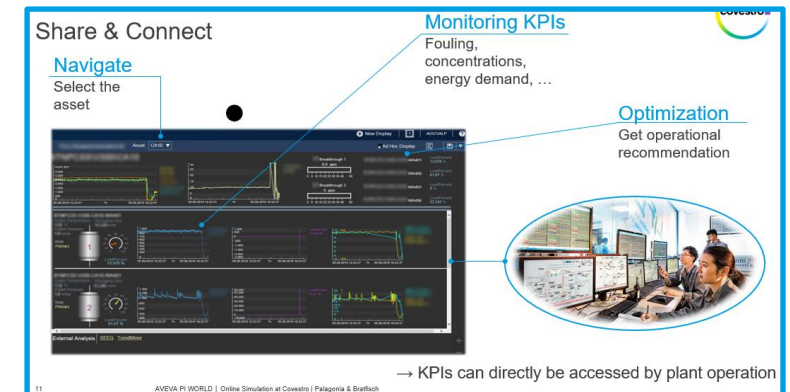
## Set-up & Maintenance

- OM set-up & roll out should be easy and straight forward from existing models
- Reduce maintenance and troubleshooting effort



## Effective Usage

- Important results should be accessible using established tools/ways
- Transparent documentation of OM status and run history
- Advanced model/process monitoring





# Different Simulators – Different OM Features & Workflows

```

3. Iteration -----<Conti>-----1.000000 *
4. Iteration -----<Conti>-----1.000000 *
5. Iteration -----<Conti>-----1.000000 *
6. Iteration -----<Conti>-----1.000000 *

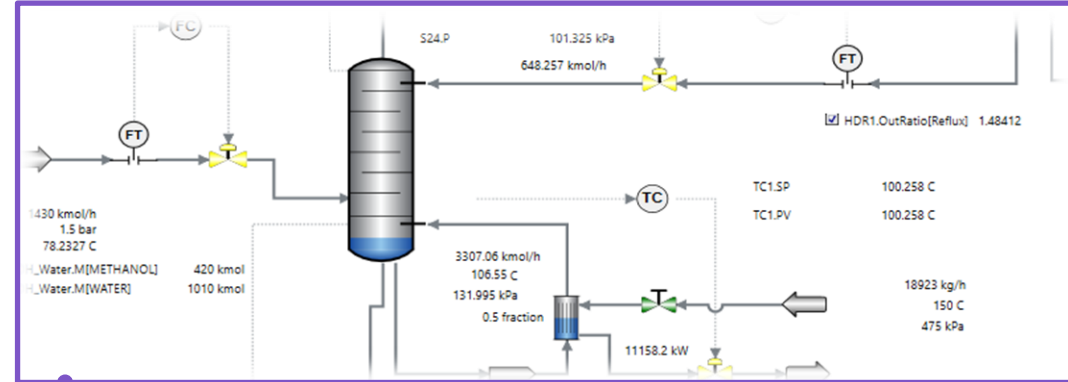
FILL
QUIT

PROPERTIES COND; COMPONENTS 2      ! Stoffdaten von Wasser und
                                   ! und Stickstoff

NEED; ENTHALPIE IDEAL;
USEQ TDEAT;
  
```

## In-house Simulation (VtPlan):

- No graphical user interface
- Troubleshooting OMs cumbersome
- Complex maintenance of PI data connection  
→ Additional tools and files necessary
- Constraints if used beyond Covestro's established core processes



## Aveva Process Simulation:

- Graphical user interface
- Python interface to control models
- Built-in connection to PI data
- Additional features, e.g.,
  - Electrolyte thermodynamic
  - Optimization
  - Specification switch (fixed, free)

# Model Configuration and Integration

- Traditional model configuration: Using text files
  - Additional tools needed to connect PI data, get an overview and insights
  - Separate file(s) needed for each model
- New approach: Using PI-AF
  - Simulated & measured values, model configuration and status in one place
  - Apply models quick & easy to additional assets (same type) using templates

```
<model name="BPA_Reactor" independent="true">
  <modelfile>BPA_Reactor.ctl</modelfile>
  <dummyfile>NoInput.ctl</dummyfile>
  <protpifile>pidata.txt</protpifile>
  <myvaroutfile>myvar.out</myvaroutfile>
  <resultfile>vt_plan_result.xml</resultfile>
  <statustag name="R2_STATUS.VTPLN" />
  <variables>
    <variable name="cAcetone" description="Acetone concentration" unit="%" tagname=
      " " default=""/>
    <variable name="cWater" description="Water concentration" unit="%" tagname=
      " " default=""/>
    <variable name=" " description=" " unit="ppm" tagname=
      " " default=""/>
    <variable name="cSolids" description="Solids concentration" unit="%" tagname=
      " " default=""/>
    <variable name="cIso" description="Isomer concentration" unit="%" tagname=
      " " default=""/>
    <variable name="TempIn" description="Rx inlet temperature" unit="°C" tagname=
      " " default=""/>
    <variable name="FlowIn" description="Reactor 2 feed flow" unit="M#/HR" tagname=
      " " default=""/>
    <variable name="ACBT" description="Reactor 2 acetone breakthrough" unit="%" tagname=
      " " default=""/>
    <variable name="Press" description="Reactor 2 pressure" unit="psia" tagname=
      " " default=""/>
  </variables>
</model>
```

History of non-PI data

Date1	Exchange Number	Reactor Catalyst Volume
	0	
	1	
	2	
	3	

Simulation file

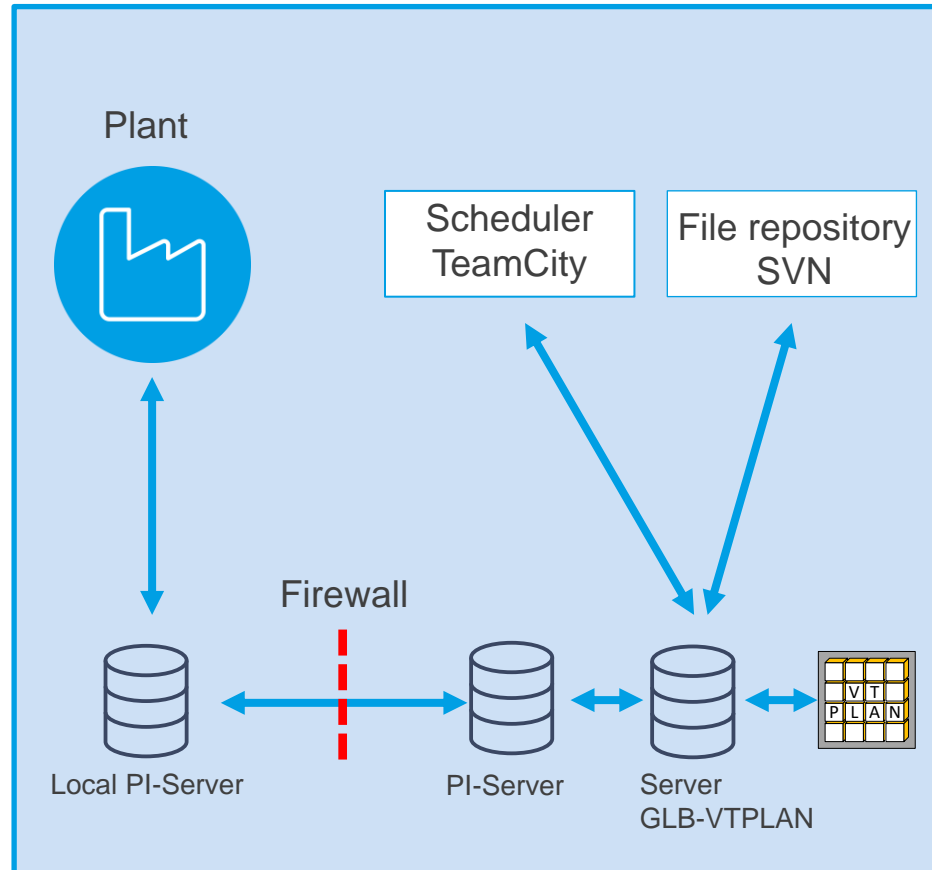
Label

Variable type & name in simulation

Filter

Name	Value
Category: 01-User Specified Asset Information	
Maximum Flow	
Minimum Flow	
Reactor Diameter	
Reactor Height	
Reactor Number	
Reactor Status	
Reactor Volume	
T-Position	Double Array
VtPlan setup	
Averaging Period	24
ModelFile	BPA_Reactor_...ctl
PRDBProject	R1
PRDBVersion	1
Reference Tag	Breakthrough
Category: 02-User Specified Constants for Process Calculations	
Density	
Fresh catalyst Volume	
MW Reactor Inlet	
Category: 03-User Specified Measurements from PI Points	
Category: 04-PI Points Mirrored	
Acetone Concentration Inlet	
Simulation Variable	Input/cAcetone
Tag Name	
concentration Inlet	
Concentration Inlet	
centration Inlet	

# Established Infrastructure



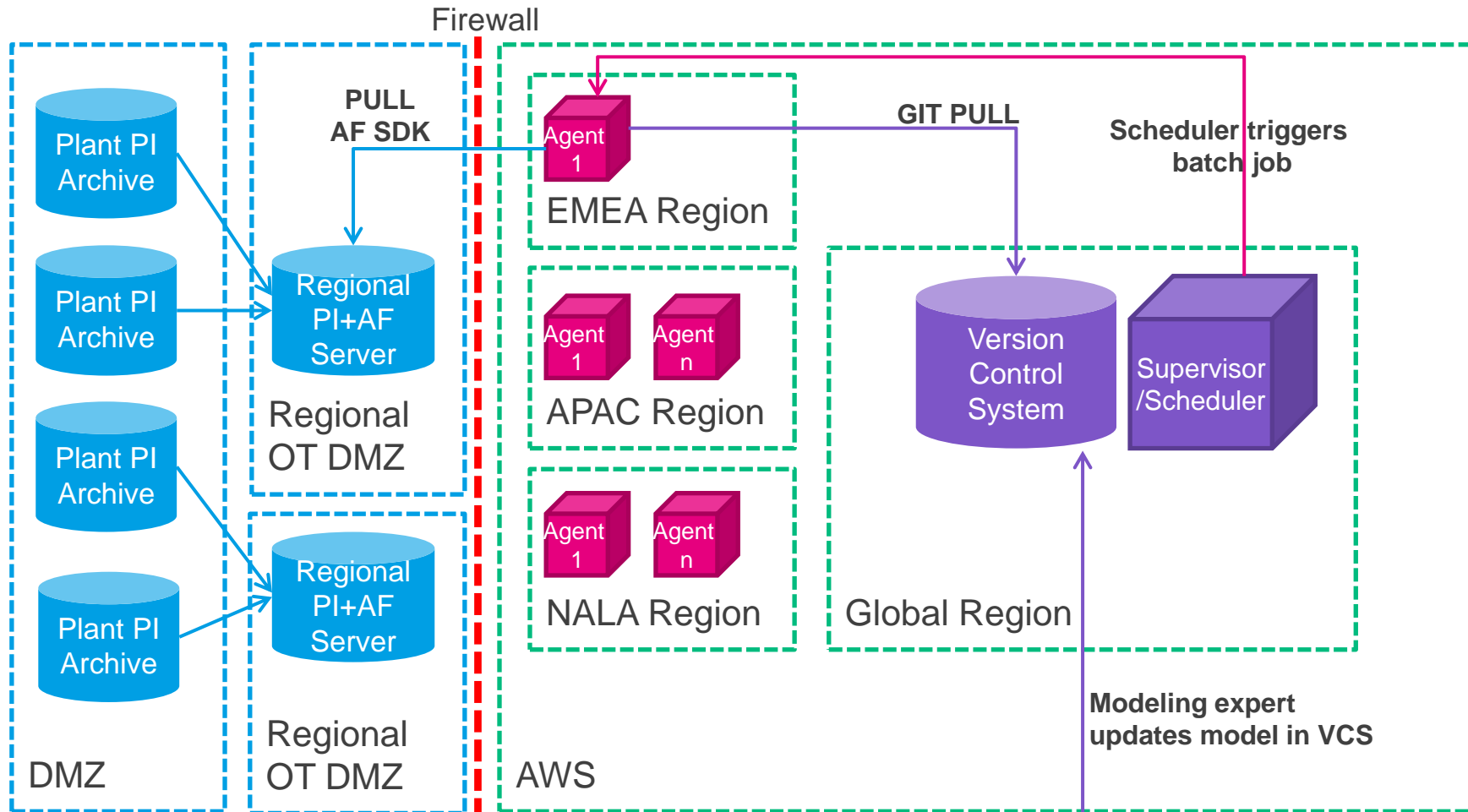
- All systems on-prem
  - Scheduler, repository (model files & configuration files), model runners hosted on a single machine
- Not flexible, scalable or extensible
- Single point of failure



**Live**

Executing  
right now!

# Proposed New Architecture (DRAFT)



Arrows indicate causality of data-transfer, arrow points from initiating system to receiving system

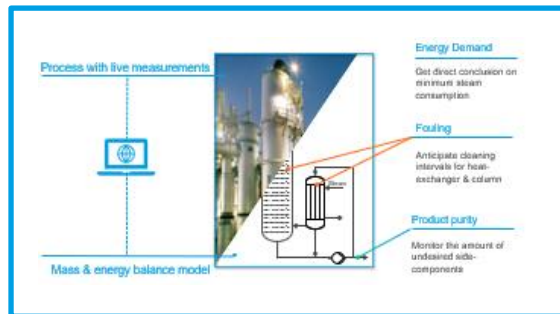
## Execution Model (DRAFT)

1. Model run gets triggered (scheduler, on demand)
2. Starting and configuring of VM
3. Download of model file(s) from VCS
4. Retrieval of needed PI data from regional servers
5. Starting the specified simulator and feeding in the data
6. Storage of most important results on the regional servers

# Online Simulation at Covestro

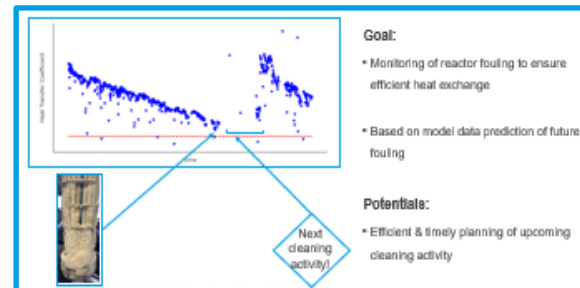
## Potential

- Process insight
- KPI monitoring for planning operations



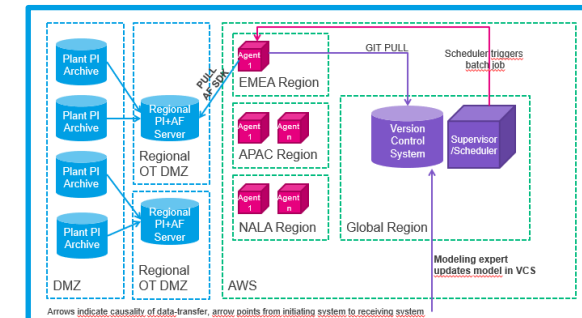
## Use Cases

- Reactor fouling monitoring
- Reactor catalyst deactivation monitoring



## Architecture

- Reduce efforts/overhead
- Transition from in-house to cloud infrastructure
- Change from file based to PI-AF based configuration






# Forward-looking statements


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