



Advancing Sustainability of Process Industries through Digital and Circular Water Use Innovations

# AquaSPICE Final Conference

Digital and smart solutions for water  
efficiency management in process industries

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The AquaSPICE project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 958396.

- A Cyber-Physical System specialised to **enhance water efficiency** in the **Process Industry**
- Water efficiency enhancement is approached from three directions:

**01**

**Production chain  
enhancement**

Design and application of state-of-the-art water treatment & recovery technologies & practices.

**02**

**Diagnosis**

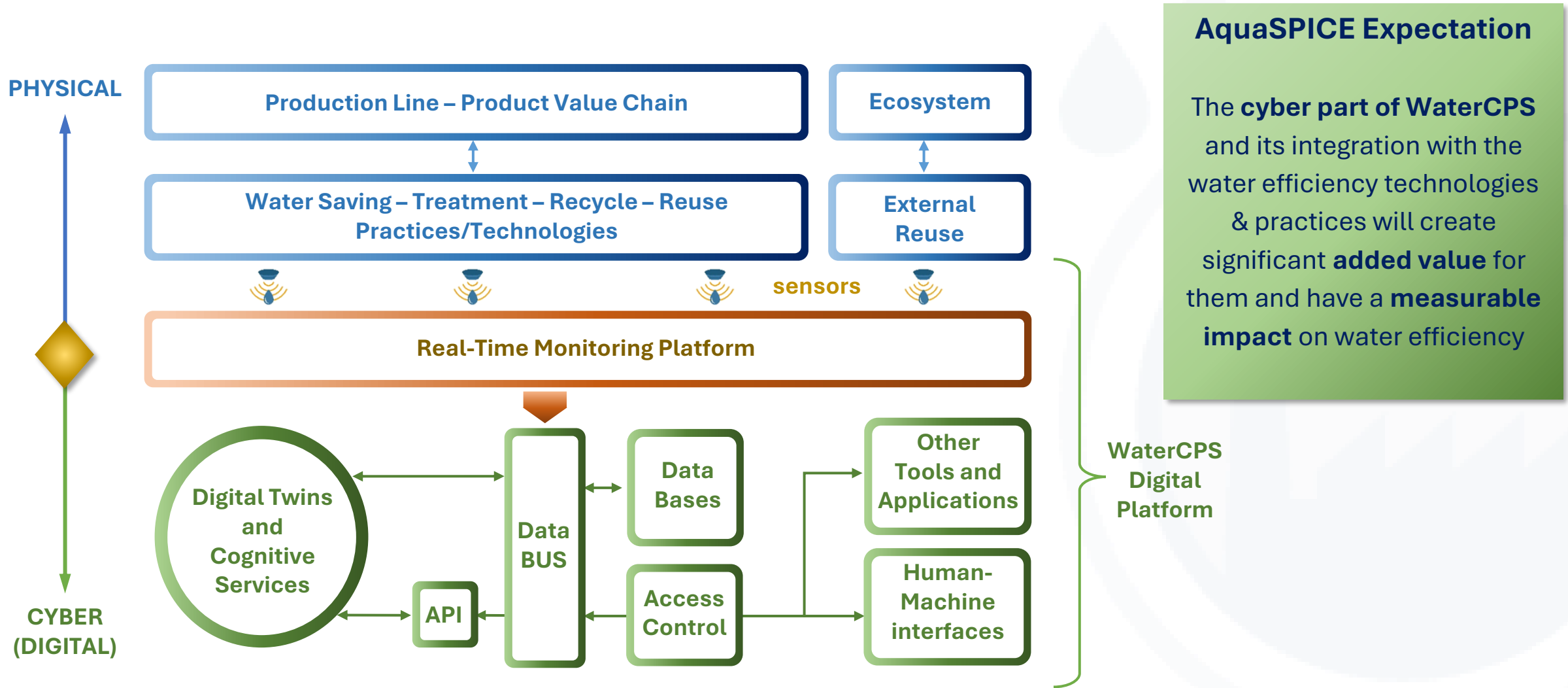
Water efficiency monitoring, issues diagnosis and improvement margins estimation.

**03**

**Optimisation**

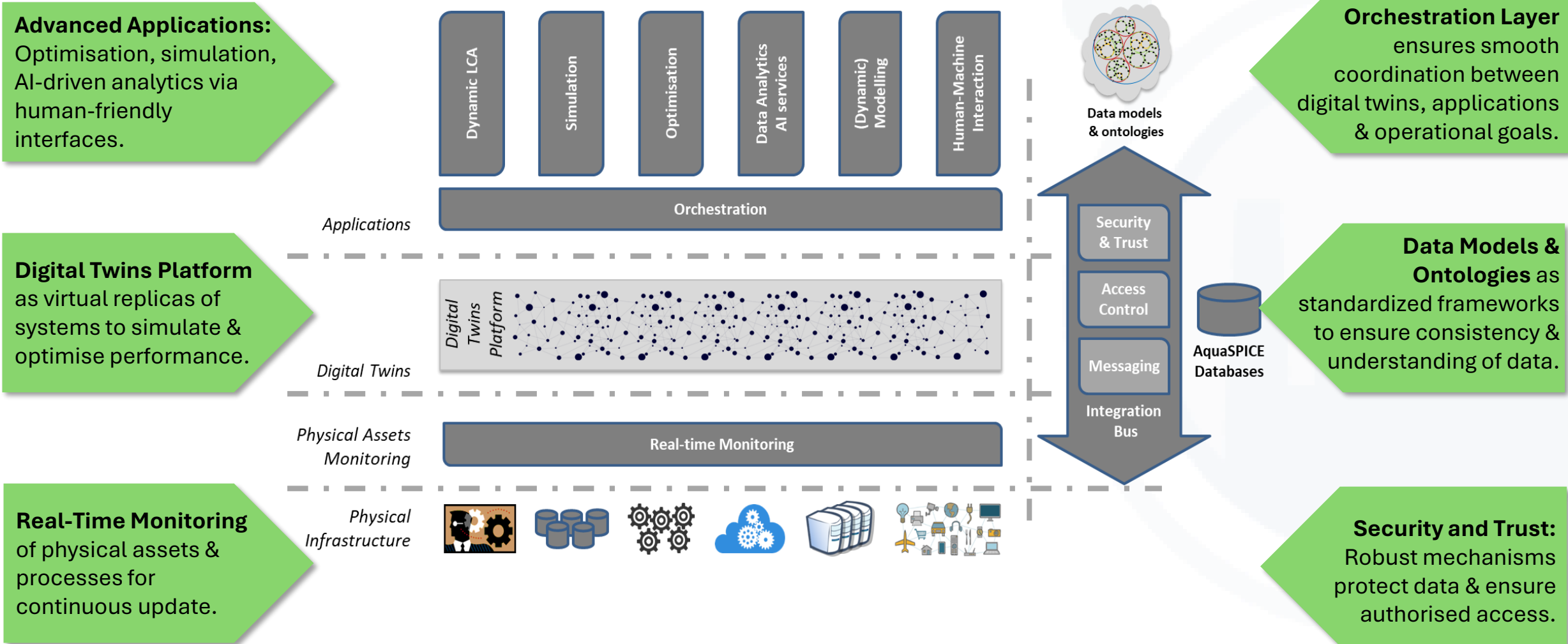
Optimise water use / recovery / reuse processes & practices.

# WaterCPS Concept

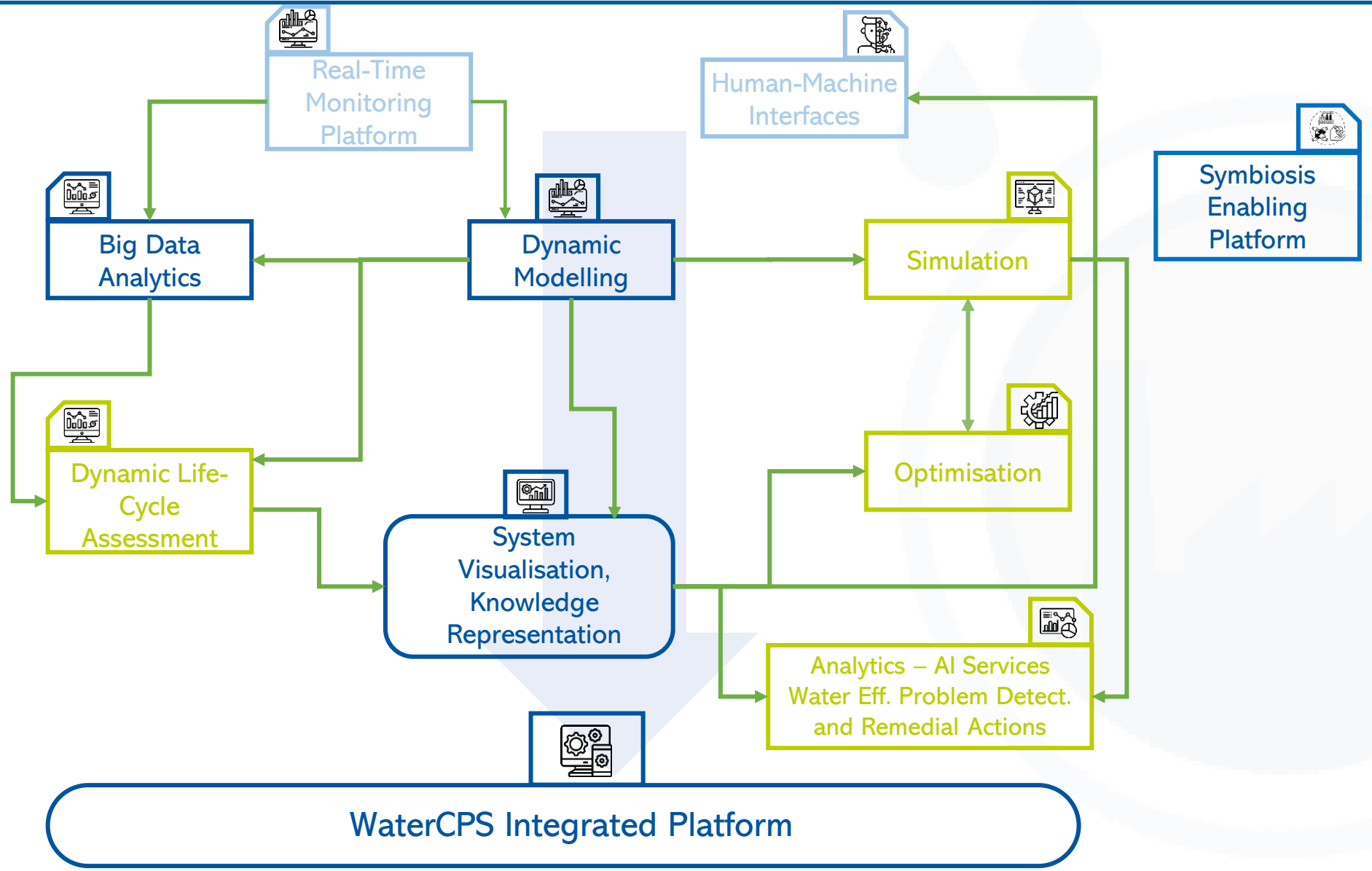


# WaterCPS Architecture

**Layered Approach:** Combines physical system, digital twins & advanced applications for a holistic solution.

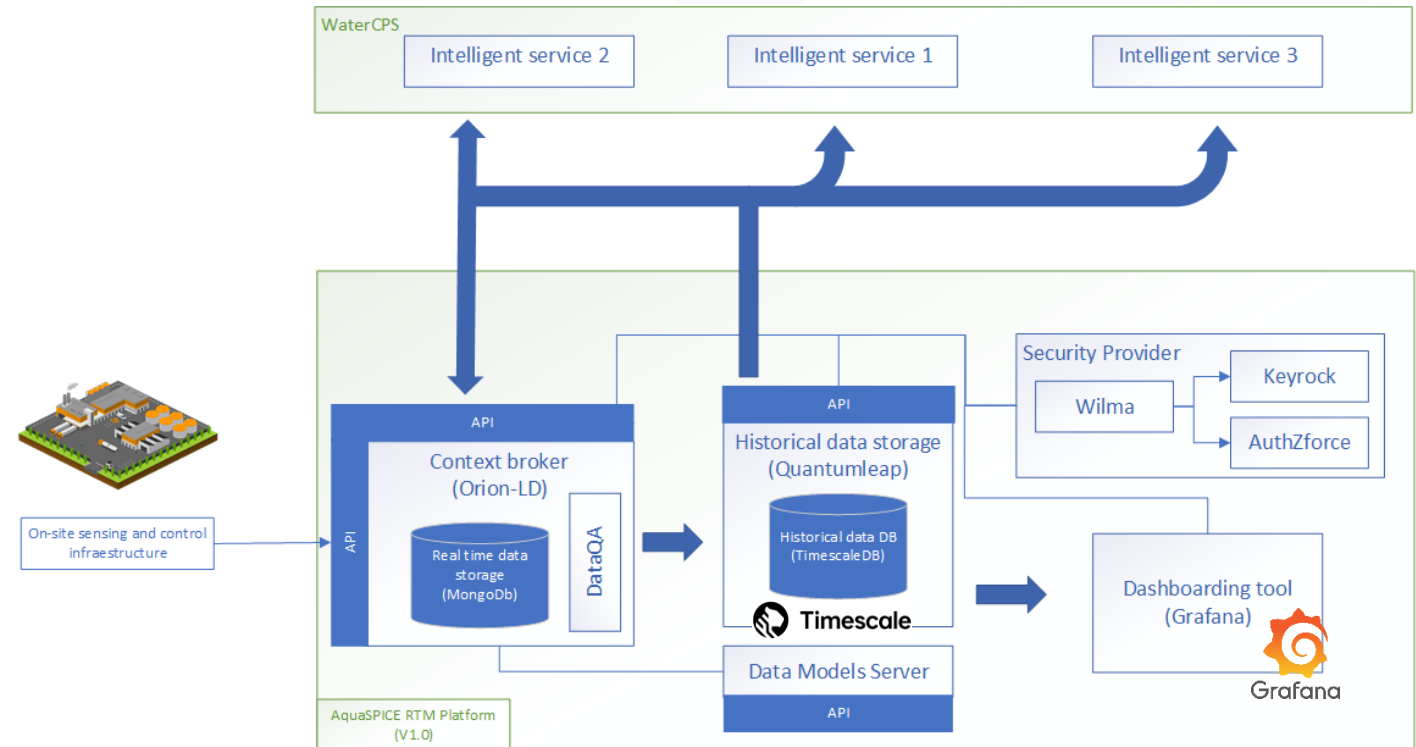


# WaterCPS Intelligence Services



## Goals:

- Collect and integrate readings from **on-site sensing** infrastructure.
- Combine data from **external sources**, such as weather reports and public water consumption metrics.
- Provide intelligent services with **access to the collected data** for analysis and decision-making.
- **Relay decisions** from intelligent services to on-site process control systems.
- Store all data **persistently** and ensure **secure access** to it.
- Enable users to create custom dashboards for **visualizing and analyzing** the data.



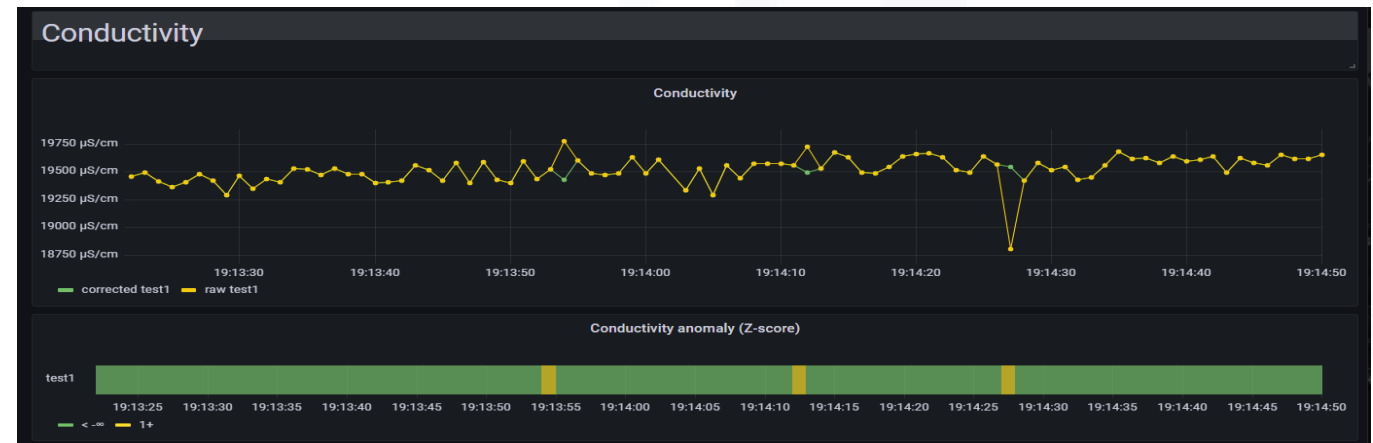
## Achievements:

- Successfully **deployed the RTM platform across 7 independent environments** for monitoring diverse use cases.
- Integrated data from **various sources** including manually sent CSV, batch sent XLS, pulling APIs, MQTT brokers, OPC-UA, etc.
- Enabling **direct interaction of the WaterCPS with the water treatment processes** (IMPROVED container)
- Implemented a **Data Quality Assurance** module, utilizing Z-score and Hampel filter algorithms ([link](#)).

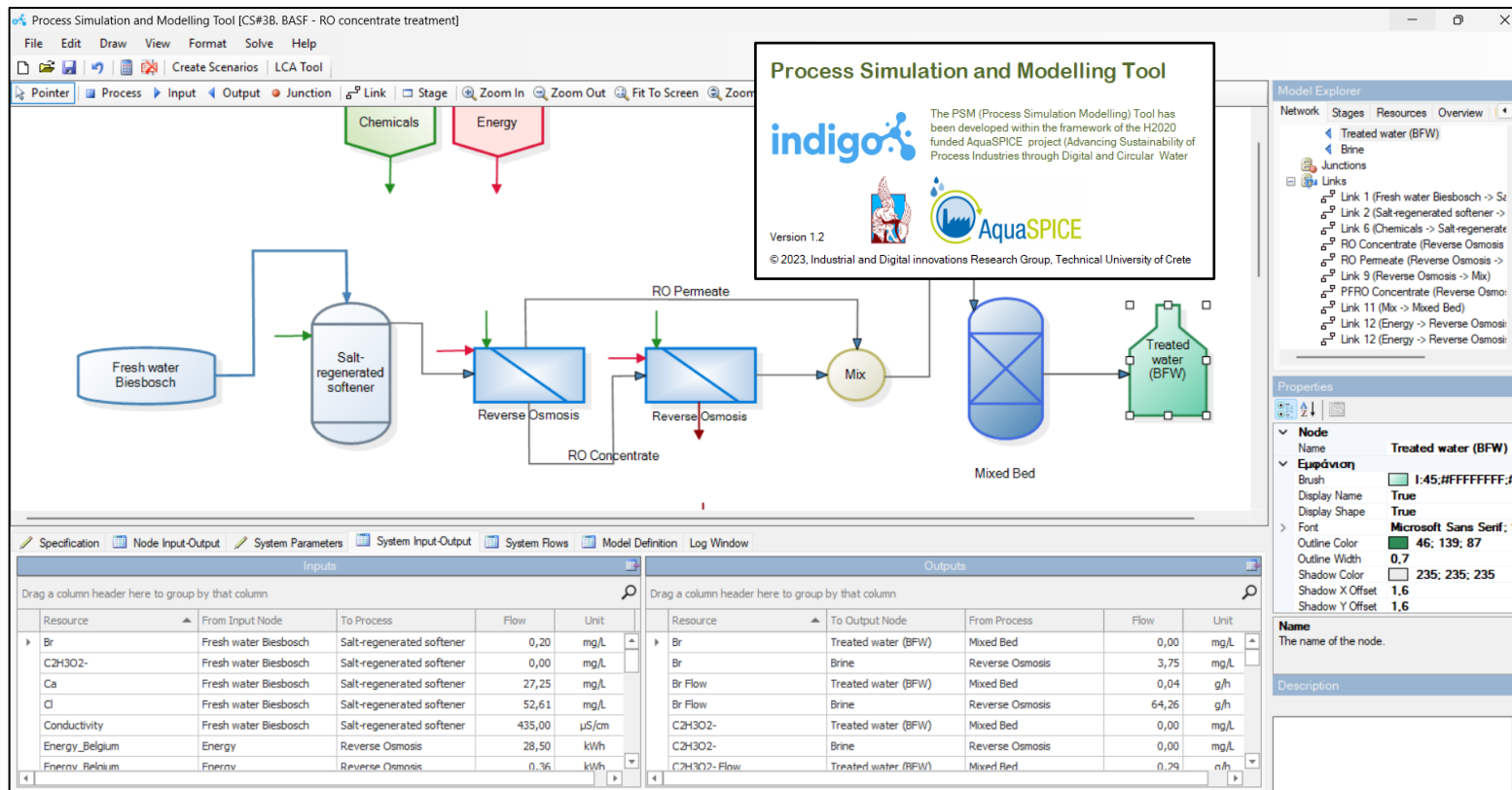
## Use Case Example: Albert canal monitoring



Dashboard of the raw data collected



Output of the z-score results of the DataQA module for the detection of anomalies in the conductivity values.



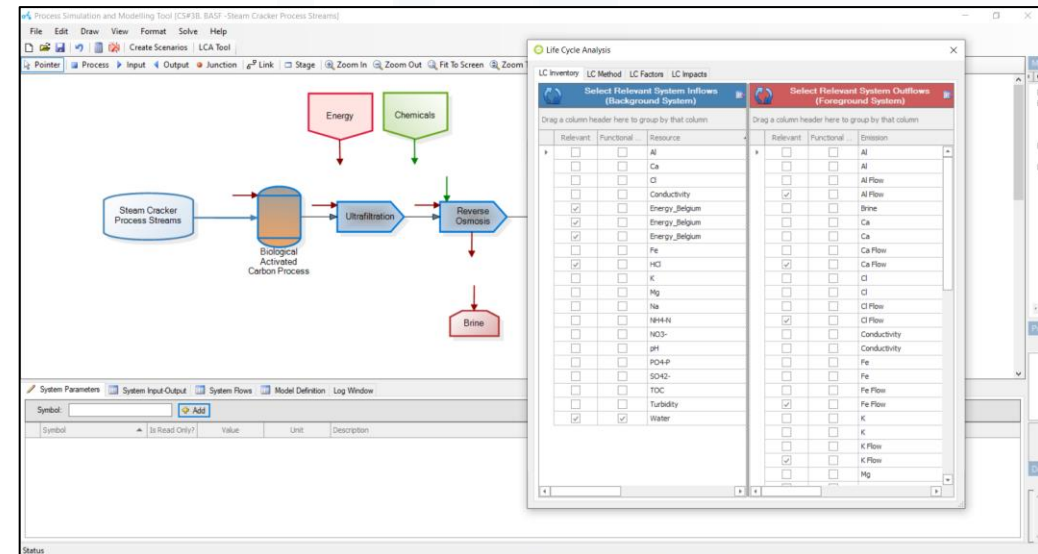
## Tool for process modelling and simulation

- ✓ Prediction of **treatment trains' performance** (quality, energy, chemical)
- ✓ Demonstration of **mass balance approach** to identify water loss
- ✓ Indication of optimal scenario in a **multi-actor system** under technological, economic and environmental criteria

- **3 modelling levels** (in-process, water balance, systemic) were identified.
- **13 mechanistic models, 2 hybrid models and 11 treatment trains** were simulated.
- **PSM-LCA tool was developed** for simulation and life cycle assessment purposes.

- The AquaSPICE Dynamic LCA framework has incorporated the following steps of a conventional/static LCA:
  - **Dynamic Goal and Scope**
    - The user can decide on the functional units and the boundaries of the system, through the PSM tool
  - **Dynamic Life Cycle Inventory**
    - The user can select the flows that will be part of the inventory, through the PSM tool
    - These flows are populated either directly, via the RTM component, or indirectly, calculated by the PSM tool
  - **Dynamic Interpretation**
    - The user can see the results and compare them with benchmark values, via the WaterCPS dashboard

- It was decided that the Dynamic Characterisation is not suitable for short-term (near real time) life cycle assessment
- The Environmental Footprint 3.0 method has been used, combining both midpoint impact indicators and a single score indicator




## Technologies

### Front-End

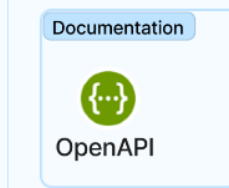


### Back-End

#### APP




#### Documentation




#### Data


##### Database



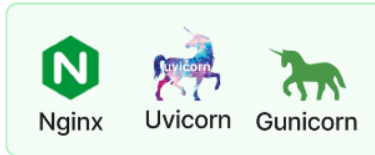
##### Messages



#### Machine Learning



### Web Infrastructure



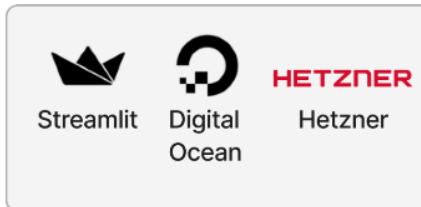
### Orchestration



### Cloud Infrastructure



### Prototyping



## Applications

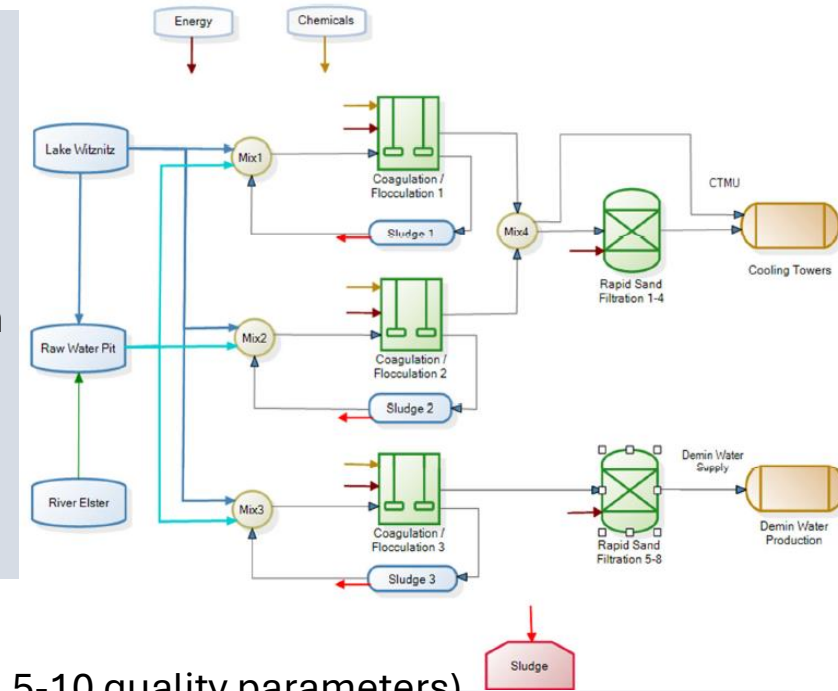
- Insights on the water streams through time-series **graphs, visualisations** and **data aggregations**
- **Virtual sensors** for the water quality of the effluent of a modular water treatment pilot plant ('MPROVED Containers)
- **Predictive analytics** to estimate water quality parameters (e.g, pH, UVAS, Nitrates, conductivity)
- **Analyses of sensor data** to identify key variables affecting water quality, e.g., pH
- **Time-series forecasting** to predict future TOC values of water streams
- Automated Analysis of **Flow Cytometry** data to identify bacterial populations or identify system faults

## Challenges

- Optimize network flows, while respecting multiple strict constraints on real time decisions
- Reconfigure network flows for maintenance activities and respond to unexpected events
- Explore potential network configurations (integration of additional components or alternative connection arrangements).

## Solution

- Input: a process network consisting of
  - ✓ Various components (treatment processes, wastewater sources)
  - ✓ Their connection links and attributes, such as capacity & quality requirements
  - ✓ The optimiaation criteria (cost, energy, fresh water intake)
- Input data are automatically translated to a mathematical programming formulation solved by an exact solver
  - ✓ Generic design allows for applicability on similar flow optimisation problem
- optEngine operates online (daily or during an unexpected event) and proposes optimised flows within the network under multiple objectives and given constraints.



## optEngine Results

- Fast (near-)optimal solutions in a few seconds for various inputs (5-15 components, 5-10 quality parameters)
- Support the selection of the most cost-effective design investment.
- Improved operations with regards to critical KPIs, such as:
  - ✓ Water reuse up to 90% ( $\approx 2.3$  MCM/year) in Tüpraş
  - ✓ Water intake reduction up to 18% ( $\approx 1.2$  MCM/year) in Dow

In the WaterCPS platform all **AquaSPICE Case Studies** **deployed**, including:

- Interconnection with the RTM platform for real-time data transmission
- Inclusion of all wastewater streams that were investigated (IMPROVED containers, MERADES pilot plant, WAPEREUSE system, Fit-for purpose pilot plants)
- Digital Twins
- All process configurations
- All WaterCPS intelligence services (simulation, life cycle assessment, data analytics, optimisation)

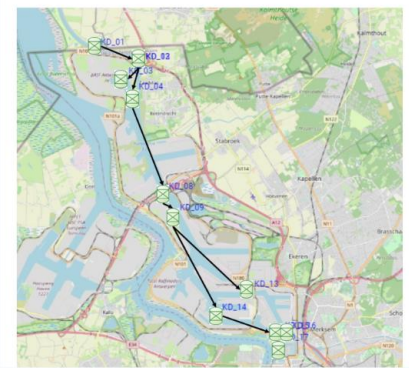


<https://portal.aquaspice.eu>

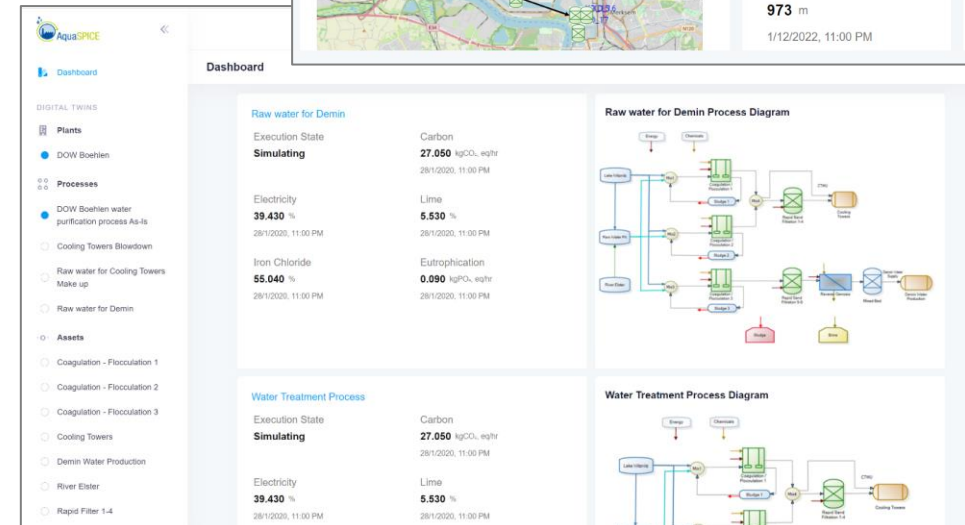
Antwerp harbor water monitoring process as-is

Execution State  
**Running**

Process Diagram



<b>KD_01</b>	<b>KD_02</b>
Depth 775 m 1/12/2022, 11:00 PM	Depth 754 m 1/12/2022, 11:00 PM
<b>KD_03</b>	<b>KD_04</b>
Depth 1273 m 1/12/2022, 11:00 PM	Depth 1133 m 1/12/2022, 11:00 PM
<b>KD_07</b>	<b>KD_08</b>
Depth 973 m 1/12/2022, 11:00 PM	Depth 1426 m 1/12/2022, 11:00 PM



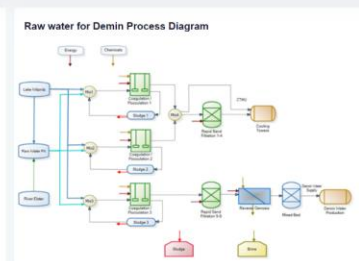
**Dashboard**

**Raw water for Demin**

Execution State  
**Simulating**

Carbon	27.050 kgCO <sub>2</sub> eq/hr
Electricity	39.430 %
Iron Chloride	55.040 %
Lime	5.530 %
Eutrophication	0.090 kgPO <sub>4</sub> eq/hr

**Raw water for Demin Process Diagram**

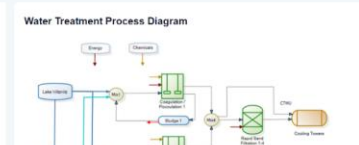


**Water Treatment Process**

Execution State  
**Simulating**

Carbon	27.050 kgCO <sub>2</sub> eq/hr
Electricity	39.430 %
Lime	5.530 %

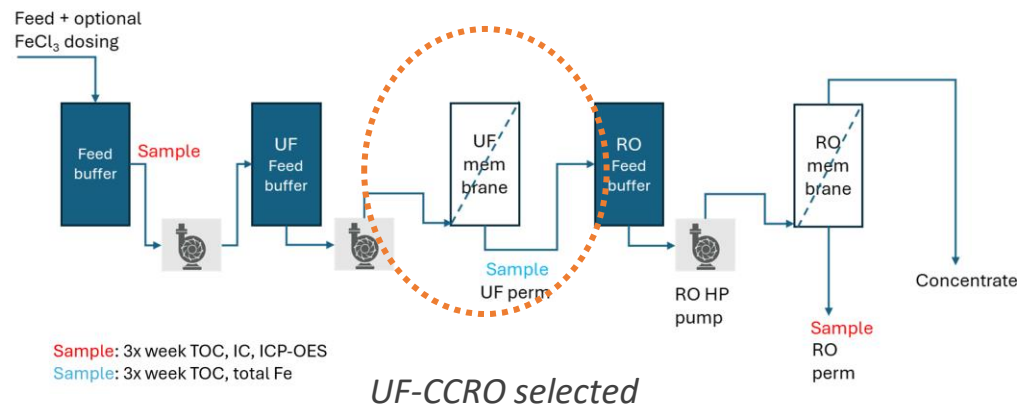
**Water Treatment Process Diagram**



## BASF WWTP effluent AND IMPROVED Pilot



1. Feasibility of reuse of WWTP effluent as process water
2. Full implementation of RTM and WaterCPS platform



  
  
 Improve performance  
 UF unit



### Full implementation WaterCPS concept

#### Applications

1. UF permeability performance
2. Determination of critical flux

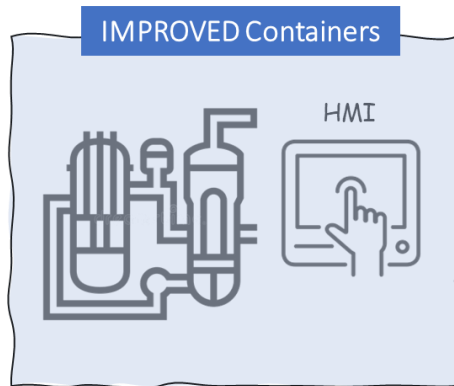
#### Functionalities

- Online data transmission to **RTM platform**
- Online connection to **WaterCPS services** (calculations, alarms, optimization loop)

## BASF WWTP effluent AND IMPROVED Pilot

### Full implementation WaterCPS concept

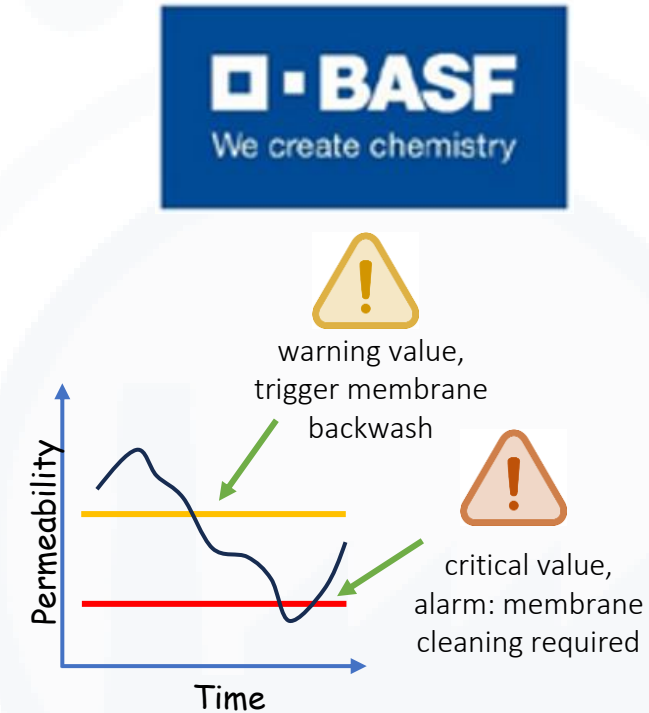
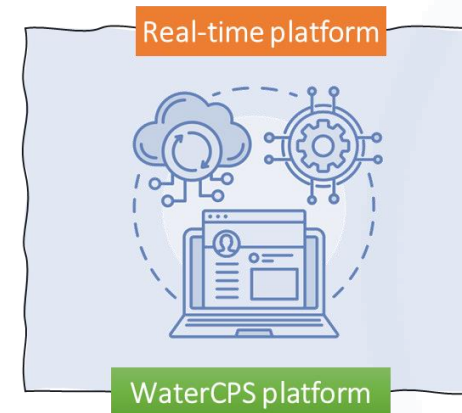
1  
UF Permeability performance



Sensor data (temp, pressure, flowrate)



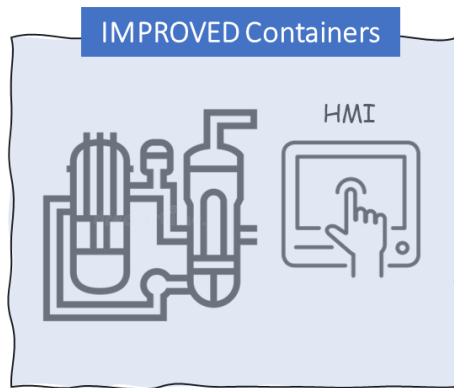
- ✓ Permeability
- ✓ Alarms in HMI
- ✓ Trigger backwash
- ✓ Cleaning recommendation



## BASF WWTP effluent AND IMPROVED Pilot



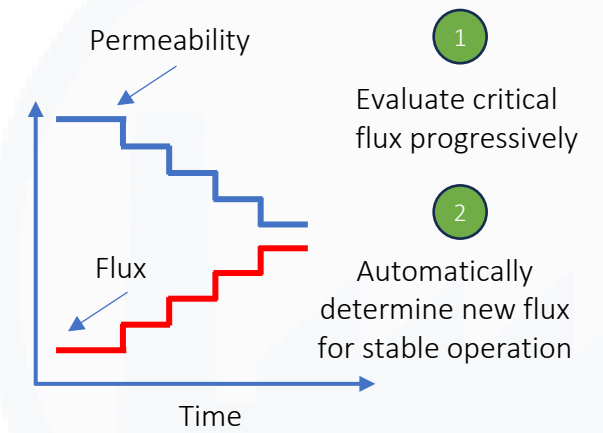
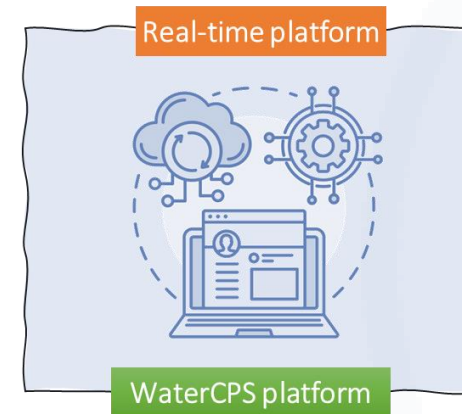
**2**  
Critical flux determination



Sensor data (temp, pressure, flowrate)



- ✓ Permeability
- ✓ Critical flux
- ✓ New flux setting



- Real time bidirectional data flow (sensors data, calculations, setpoints)
- Real time follow of UF process performance
- Generation of alarms to support maintenance (membrane cleaning)
- Automatic optimization of operational conditions



## AquaSPICE

Advancing Sustainability of Process Industries through  
Digital and Circular Water Use Innovations



Advancing Sustainability of Process Industries through Digital and Circular Water Use Innovations

# Thank you

George ARAMPATZIS, Technical University of Crete (TUC)



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