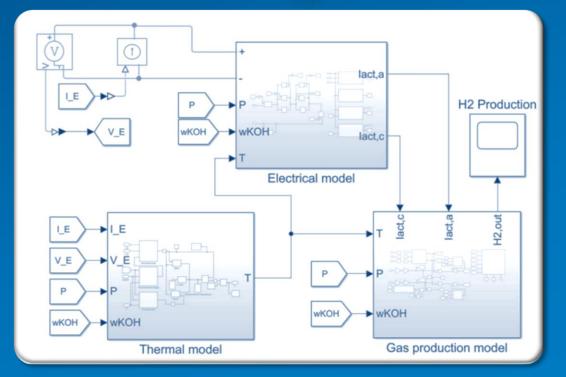


Digital Twins for New Energy Processes in MATLAB[®] & Simulink[®]



Chris R. Wells Energy Resources December 2023 (v1)





Artificial Intelligence

Big Data Deep

Learning

Analysis



Machine

Learning



Reinforced Learning



Predictive Internet Analytics of Things







Process

Digitization





Process Automation Value Chain Integration



Contents

- Background
- Digital Twins in MATLAB and Simulink
 - Types of Digital Twin Models
 - Common Digital Twin Applications
 - Digital Twin Deployment Options
 - AI-based Modeling and System Design Workflow
- Simulink[®] Digital Twins for New Energies
 - Multi-physics Digital Twins for Green Hydrogen Production
 - Modular Open-Systems Approach (MOSA) for Digital Twins
 - Optimizing Turbine Predictive Maintenance Scheduling
- MathWorks[®] Digital Twin Toolset



Background



The integration of new energy processes in the value chain requires a thorough understanding of time, cost, demand, and resources necessary to streamline these processes in the most effective and timely fashion



New energy processes comprise complex, multi-physics, dynamic systems that require comprehensive and continuous analysis and control steps to maximize data value using existing assets and allocated infrastructure



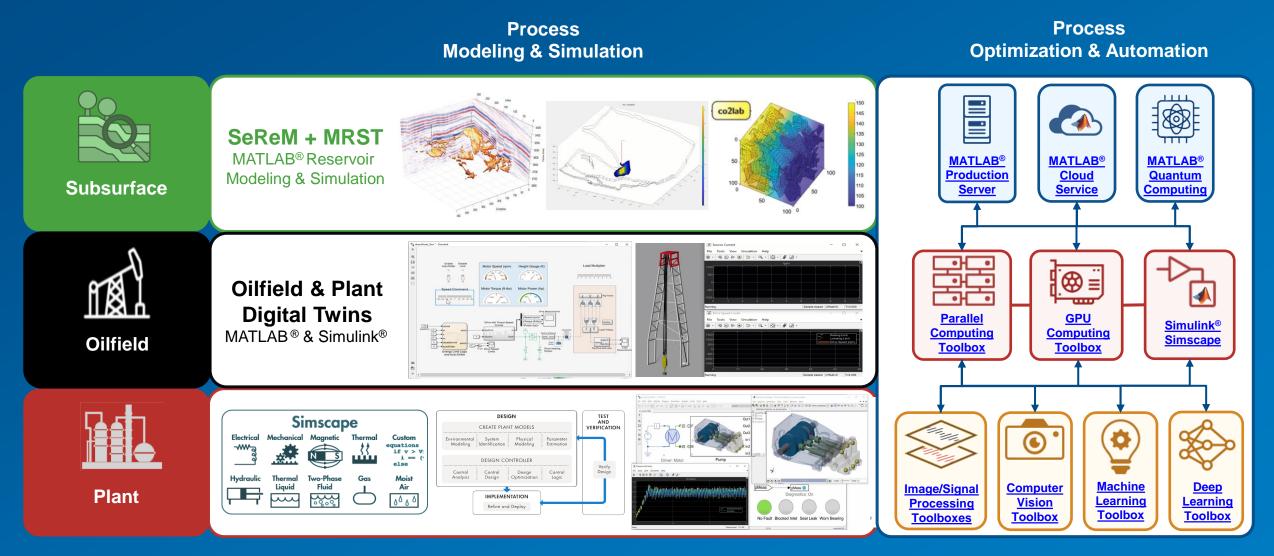
Digital twins and advanced process control (APC) are useful digital technologies for engineers, scientists, and decision makers to design, test, predict, and plan how to make the most out of a new energy process



MathWorks developed digital toolboxes in MATLAB and Simulink for organizations to build (i) digital twins that simulate dynamic systems and processes, and (ii) APC systems to maximize process performance, stability, and efficiency.



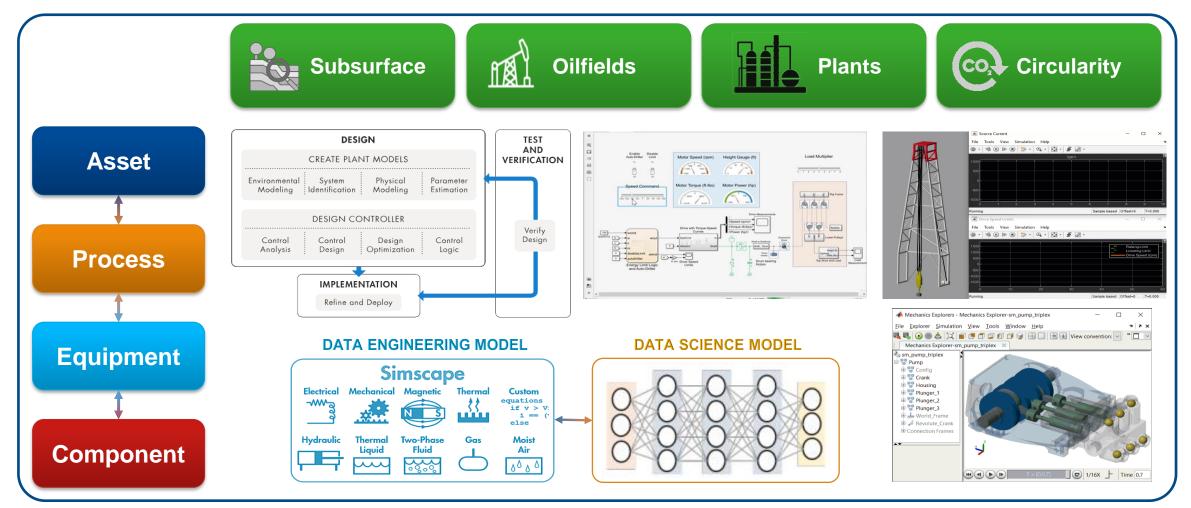
Customizable Digital Products for Energy Upstream & Downstream





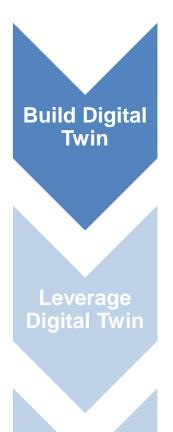
MathWorks in Energy Resources Digital Twins in MATLAB[®] & Simulink[®]

Digital Twin: A digital simulation of dynamic systems to predict outcomes and inform decisions



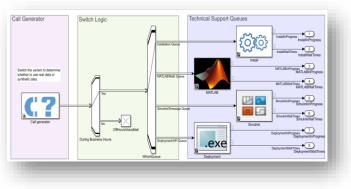


Types of Digital Twin Models

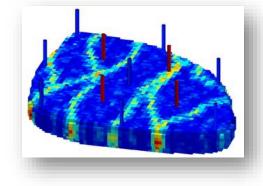


Deploy Twin & Algorithms

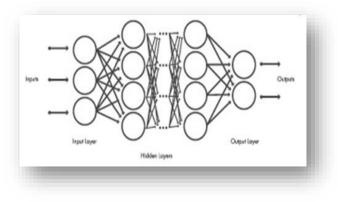
Process Model



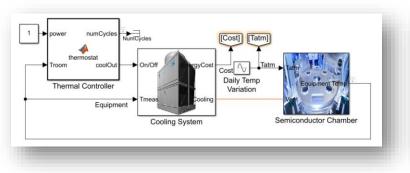
Parameter Estimation Reduced-Order Models



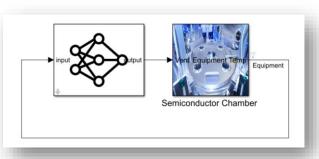
Al-based Models



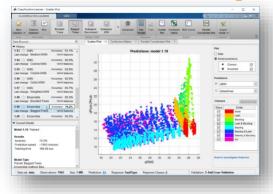
Physical Components



Hybrid Models



Machine Learning



Data-driven modeling

Physics-driven modeling



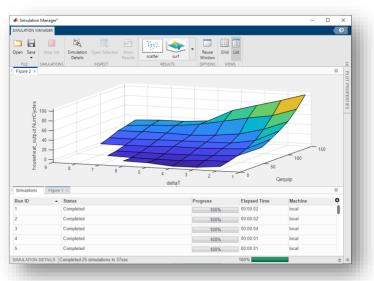
Common Digital Twin Applications

Build Digital Leverage **Digital Twin**

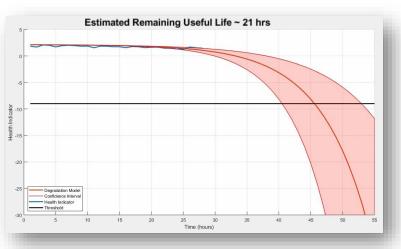
Deploy Twin &

Algorithms

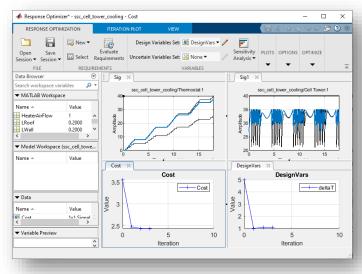
Monte Carlo Simulations

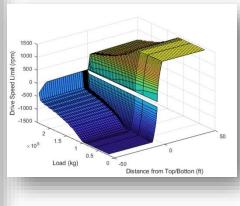


Predictive Maintenance

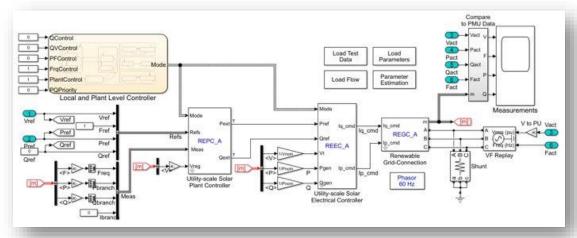


Operations Optimization





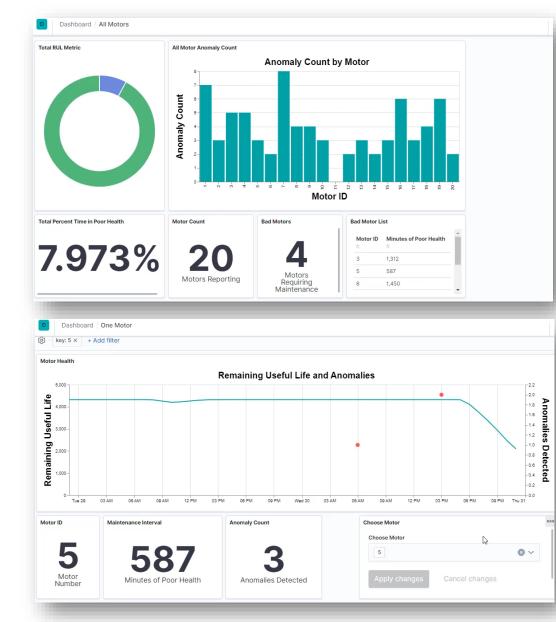
Fault Diagnostics

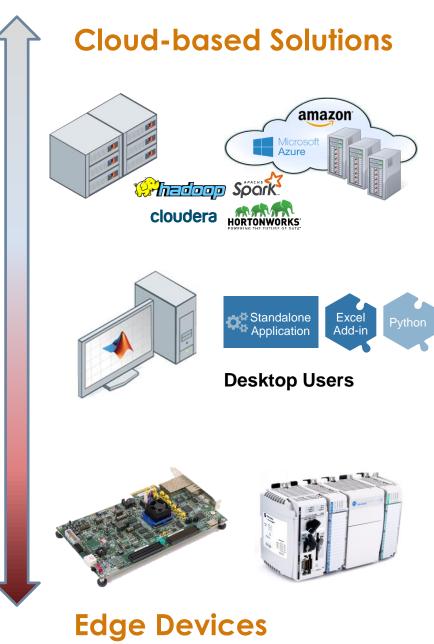




Digital Twin Deployment Options

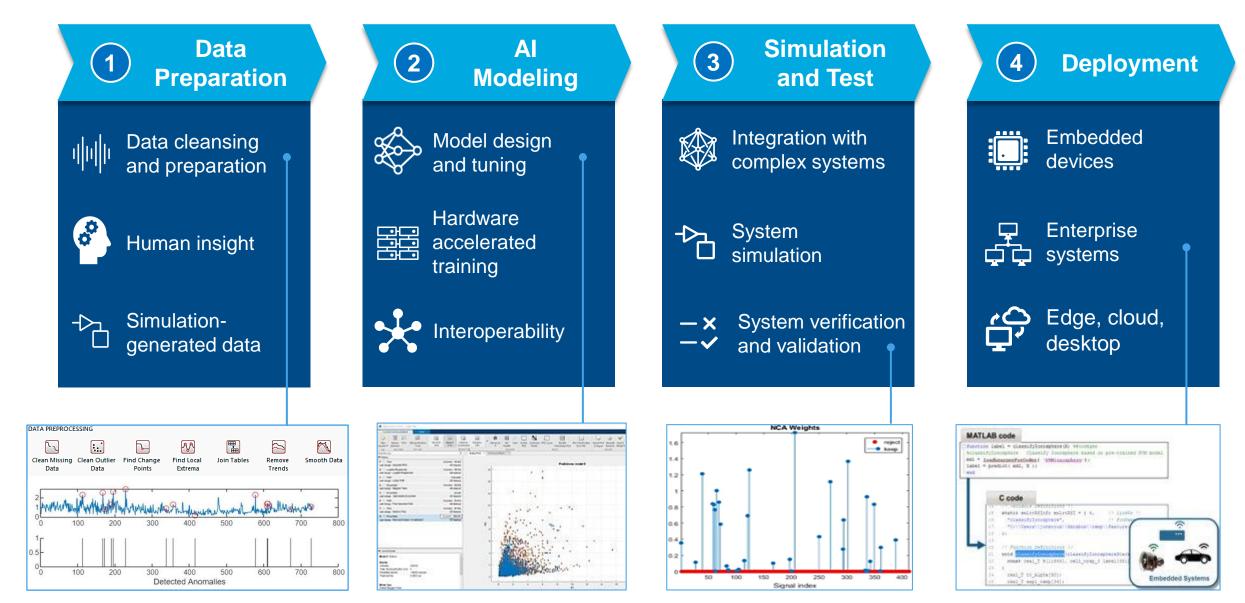








Digital Twins – AI-based modeling and system design workflow





Simulink[®] Digital Twins for New Energies

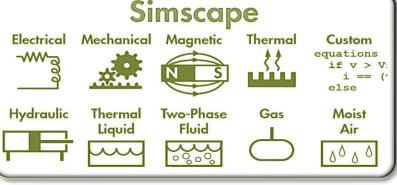
Objectives

- Model chemical reaction kinetics, thermodynamics, and mass balance across a multi-physics system of equipment components
- Integrate machine learning to develop predictive model for process testing, prototyping, DevOps monitoring, and process optimization
- Incorporate advanced control systems (ACS: PLC, DCS) and digital sensors to simulate data flow across OT/IT infrastructure (e.g., SCADA)

Case Studies

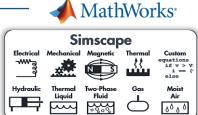
- Iribarren *et al* (2023): <u>Dynamic modeling of a pressurized alkaline water</u> <u>electrolyzer: A Multiphysics approach</u>. IEEE Transactions on Industry Applications, Vol. 59, No. 3, May/June 2023.
- Sakas et al (2022). <u>Dynamic energy and mass balance model for an industrial</u> <u>alkaline water electrolyzer plant process</u>. International Journal of Hydrogen Energy, 47, 4328-4345.
- Randall (Sasol) and Mantji (Opti-Num). <u>Predictive maintenance of a steam</u> <u>turbine</u>. MathWorks Video.

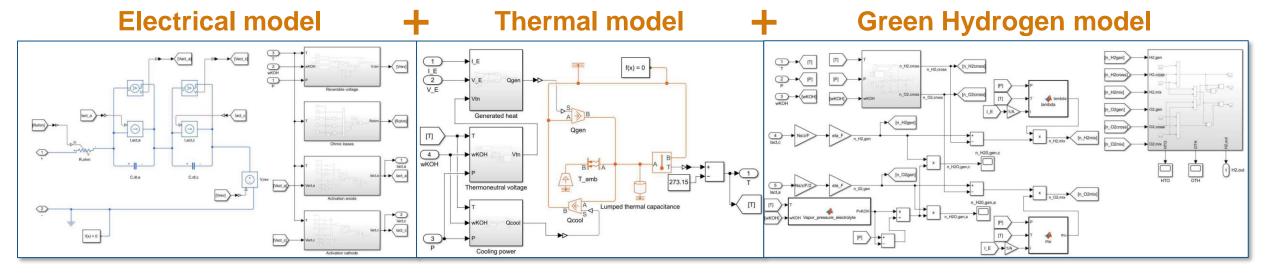




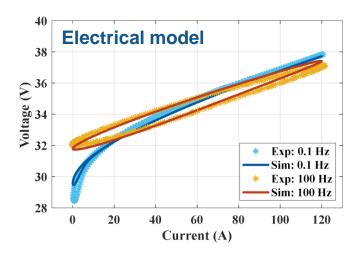
Simulink[®] Digital Twins for New Energies (Green Hydrogen)

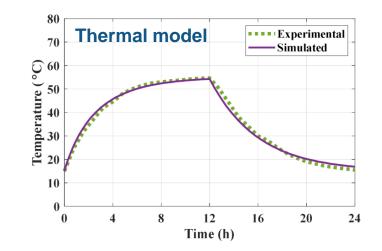
Multi-physics Digital Twin for Pressurized Water Electrolyzer (Iribarren et al, 2023)





Multi-physics verification (experiments vs. simulations):





H2 production model 2.1 1.4 × HTO_{exp}: 5 bar × HTO_{exp}: 25 bar HTO:: 5 bar _____ HTO: 25 bar 1.8 1.2 ***** HTO_{exp}: 15 bar $f_{H2,exp}$: 15 bar h-1) HTO_{cim}: 15 bar _____ f_{H2.sim}: 15 bar 1.5 ш₃ (% 0.8 0.9 OLH 0.6 flow 0.6 0.4 H₂ O. 0.2 60 100 120 40 80

Current (A)

Simulink[®] Digital Twins for New Energies (Green Hydrogen) Multi-physics Digital Twin for Pressurized Water Electrolyzer (Iribarren et al, 2023)

0.11

0.09

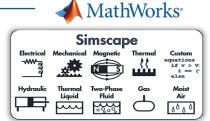
0.07

0.03

0.01

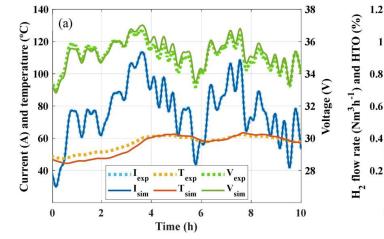
10

OTH (vol.%)



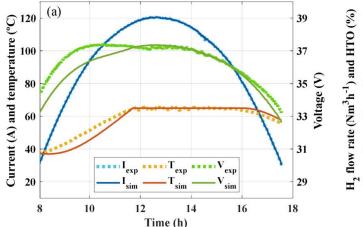
Digital twin validation – Wind Power Operation

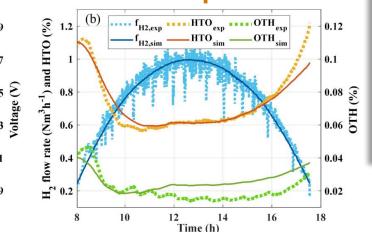
(b)



Digital twin validation – PV-based Operation

0





f_{H2.exp} ••••• HTO_{exp} ••••• OTH_{exp}

-OTH

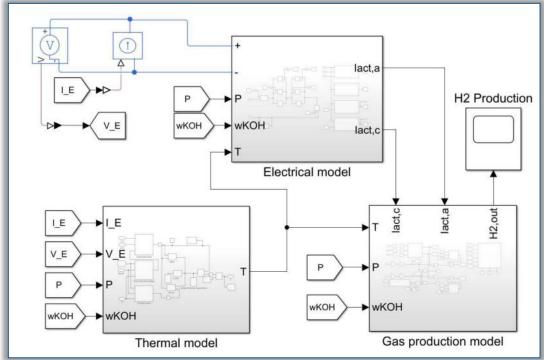
8

- HTO

Time (h)

H2.sim

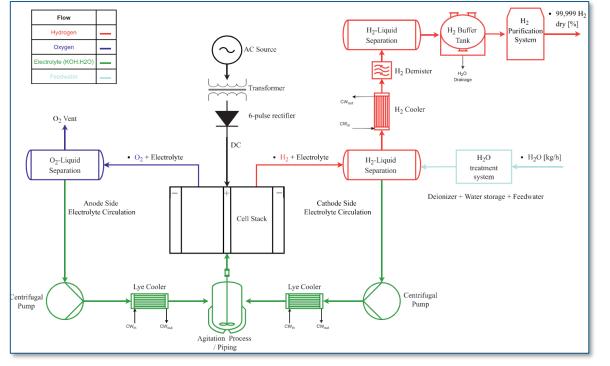
Digital Twin for Green Hydrogen Final Model



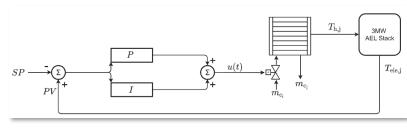


Simulink[®] Digital Twins for New Energies (Green Hydrogen) Multi-physics Digital Twin for Pressurized Water Electrolyzer (<u>Sakas *et al*</u>, 2022)

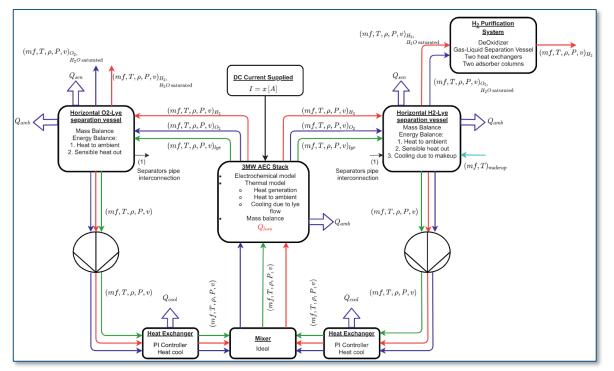
Alkaline water electrolizer process diagram



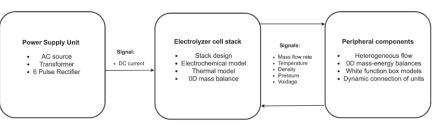
Simulink model – Cooling water feed valve control



Alkaline water electrolizer – Simulink model



Conceptual dynamic simulation model





Fluid

Custom equations if v > V: i == (' else

Moist Air ≬≬≬≬

Electrical

Liquid

لتس

₽₽₽

Simulink[®] Digital Twins for New Energies (Green Hydrogen) Multi-physics Digital Twin for Pressurized Water Electrolyzer (<u>Sakas *et al*</u>, 2022)

DC current supply and H2 production in operational time of 24 hours

10

Plant normal operantional time [hours]

Measured H2 production [Nm3/h] Measured DC Current supply [A] H2 supply

20

Multi-physics verification (measured vs. simulated):

Measured at 70 [°C]

Measured at 61.15 [°C]

Simulated at 61.15 [°C] Simulated at 59.6 [°C]

Measured at 59.6 [°C] Simulated at 70 [°C]

0.3

60

U-I curve

Polarization

0.05

0.1

0.15

Current density [A/cm²]

0.2

0.25

19

1.8 2 10 1.7

1.5

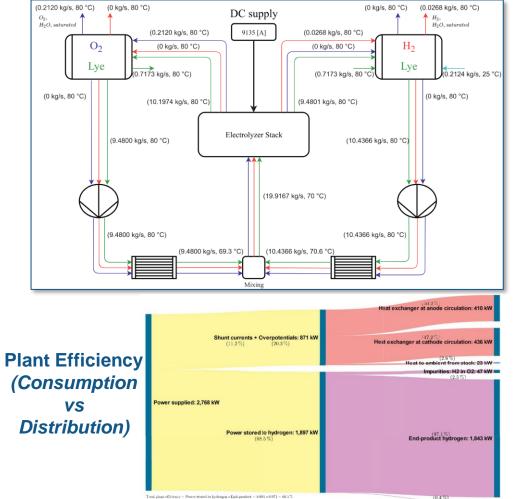
1.4

1.3

Measured vs modelled H, production Measured vs simulated stack cell temperature H2 supply 80 65 Accuracy = 98.7 % Ê 60 **Temperature** Error = 1.3 % Model/Simulation, n = 1 Model/Simulation, n = 0.86 - 3 MW Plant - 3MW Plant Simulation with Q_{shunt} - Simulation without Q 6000 6500 7000 7500 8000 8500 9000 10 15 20 DC Current [A] Operational time [hour]

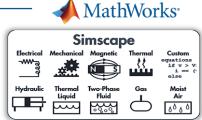
0.35

Digital Twin mass flow rates



Faraday has - (Shunt currents + Imparities + DeOxO lon) + 100 / Power supplied - 13.1 %

14



MathWorks*

MathWorks[®] in Energy Resources Modular Open-Systems Approach (MOSA) for Digital Twins

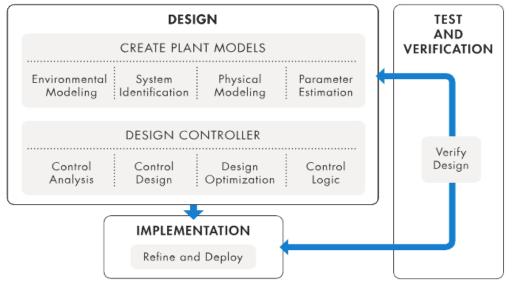
Objectives

- Monitor, predict, and automate IT/OT systems
- Integrate data science and engineering analytics

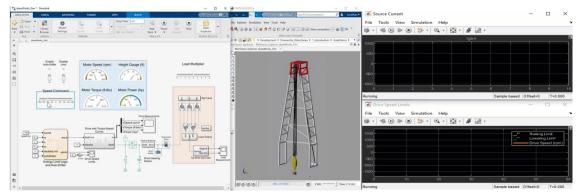
Advantages

- Full traceability and interoperability of DevSecOps
- Efficient, secure, and high-quality outputs
- Verify, adapt, and transform before you invest

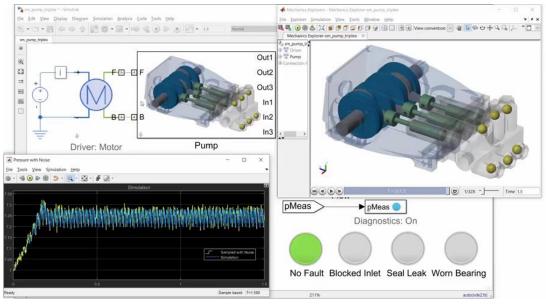
Modular Open-Systems Approach



Digital Twin for Drilling Rig Automation



Digital Twin for Pump Predictive Maintenance





Optimizing Turbine Predictive Maintenance Scheduling





sasou

Goal: Analyse performance of past maintenance and predict future efficiencies in only 100 engineering hours.



Challenges: Using historical data to detect unlogged maintenance and detect patterns that indicate efficiency of maintenance.

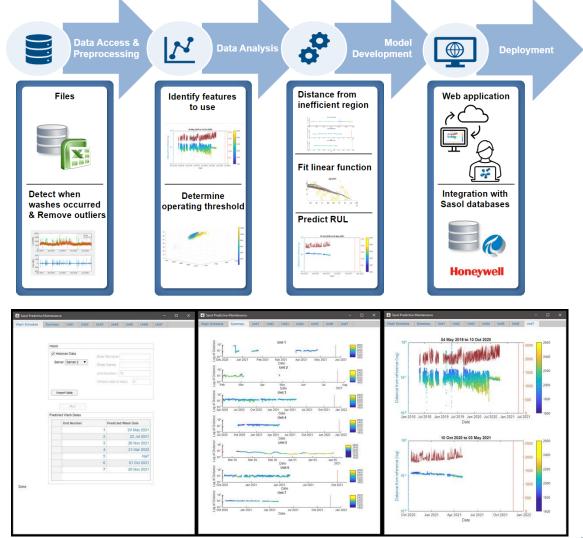


Solution: Predictive model to indicate an efficient maintenance schedule. Develop a frontend that allows operations staff to track the effects of inefficient maintenance.

Problem statements

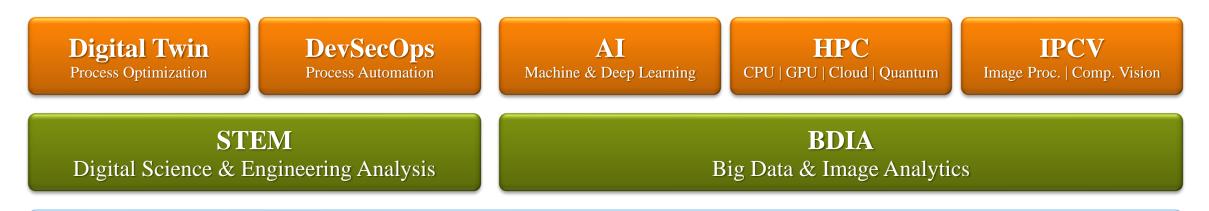
- 13.5MW condensing steam turbine @ 6,700 rpm
- 7 compressor-turbine trains | WCP: 1,600-2,550 kPa
- Plan and predict fouling within a year
- Optimize turbine performance h-s & T-s

Predictive Maintenance Workflow and Deployment





MathWorks[®] Digital Twin Toolset



$MATLAB^{\mathbb{R}} \& SIMULINK^{\mathbb{R}}$

Key technology differentiators

- Customizable STEM and BDIA toolboxes developed and fully interconnected on MATLAB[®] platform
- Model-based and data-driven science & engineering workflows to maximize data & image usage
- MathWorks[®] support, training, and development of data science, engineering, and analytics solutions
- Adaptive digital solutions to assess and integrate new energy processes using high-end technologies
- Low-cost, high-quality software solution to maximize technical expertise, IT infrastructure, and budget
- 200+ energy companies globally currently use MATLAB[®] solutions across upstream and downstream





