OCTOBER 26, 2023

Hybrid Simulation with AI

James Kattapuram | R&D Director | Simulation

Jochen Steimel | R&D Product Owner | Simulation

JC Lee | Principal Engineer | Tech Support

David Smith | Principal AI Engineer | AVEVA AI CoE

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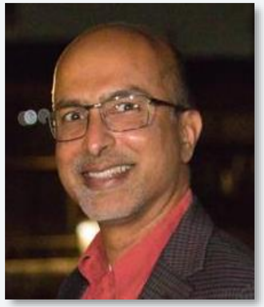

James Kattapuram

R&D Director Simulation Design Applications

James holds a MS in Chemical Engineering from University of Southern California.

James has over 25+ years' experience in developing and leading Software R&D teams, to develop next generation Simulation, design and optimization applications.

Dr.-Ing. Jochen Steimel

Simulation Platform Partner Product Owner/ Architect

Dr. Steimel holds a PhD in Chemical Engineering from TU Dortmund University.

In the first stop of his career, he worked at a German chemical company and was responsible for developing and maintaining an in-house simulator and was involved in digital/cloud/AI projects.

Since joining AVEVA, Dr. Steimel is developing the product vision for AVEVA Process Simulation (our next-generation simulation tool) and supports the R&D team with domain expertise.

Dr. JC Lee

Senior Principal Engineer

Dr. Lee holds a PhD in chemical Engineering from Yonsei University in Korea.

He started his career as a process engineer at Daelim Engineering, a Korean EPC company, working on process design, simulation, EPC projects and developing licensing technologies.

Afterwards, He joined in SimSci division of Invensys and has contributed SimSci business at presale team and technical support team. He now leads APAC SimSci technical support team.

Dr. David Smith

Principal AI Engineer,
AI Center of Excellence

Dr. Smith is a Chartered Mechanical Engineer and holds a Ph.D. in Fluid Mechanics from Imperial College London

Spending the first half of his career in industry mainly with EPC companies; he led design, development, and commissioning of Power Plant processes and combustion systems. Moving to AVEVA, Dr. Smith joined the AI Center of Excellence, where his main activities are the integration of AI technologies with AVEVA's first principles simulation products for asset management and autonomous operations.

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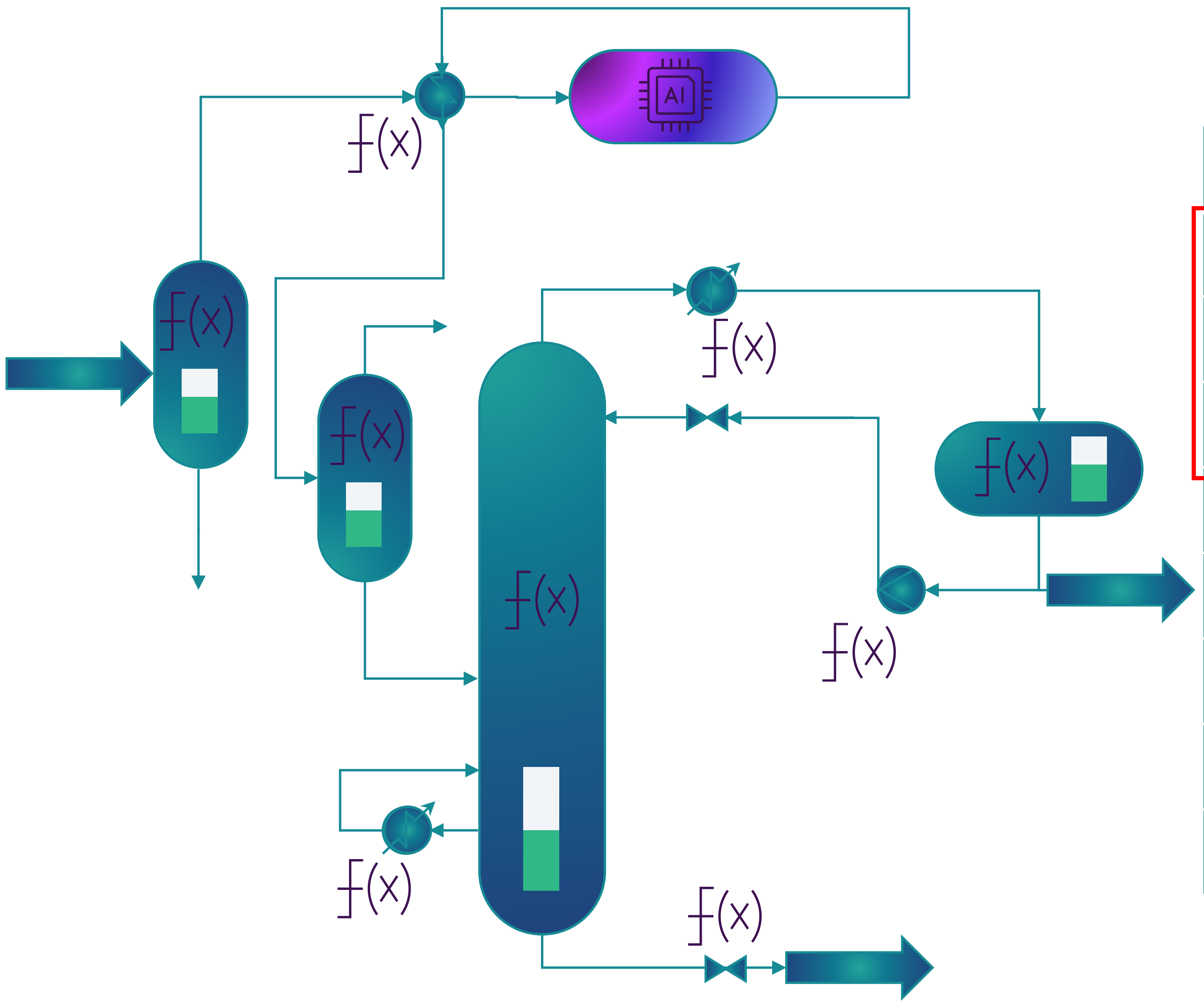
Agenda

- Introduction to Hybrid Modelling
- Hybrid Modelling in AVEVA™ Process Simulation 2023
- Lighthouse Customer Use Case: ISU Chemicals

Hybrid Modelling



Equation Based Model	ML Model
Advantage	**Limitation**
Accurate calculation of typical equipment	Time consuming to generate model
Prediction of untried operation	Prediction within data range
Acquisition of required data for design	Hard to calculate all required data for design
Limitation	**Advantage**
Difficult to obtain kinetic data for reaction	Accurate reaction prediction from actual operating data
Need extra equation for special equipment	Prediction of any equipment by using actual operating data
Limited by available thermodynamic properties data	Applicable for any properties from actual operating data
Complex problems may be slow to converge	Can be faster to solve

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Hybrid Modelling

What is a machine learning model?

PI Server

	A	B	C	D	E	F	G	H	I
1	Timestamp	Q1012	Q1013	Q1014	TT102	PT476	Q2032	Q3034	TT8178
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3	25/09/2023 01:00	0.346322	1.801618	0.788249	321.0969	26.03024	1.523908	0.738202	298.2171
4	25/09/2023 02:00	0.529183	1.755596	0.768752	321.2447	25.88786	1.535431	0.682269	298.2202
5	25/09/2023 03:00	0.583307	1.910638	0.845692	320.8985	26.20656	1.487193	0.639415	298.0486
6	25/09/2023 04:00	0.228065	1.639018	0.670427	320.9417	26.02546	1.402999	0.694899	297.9373
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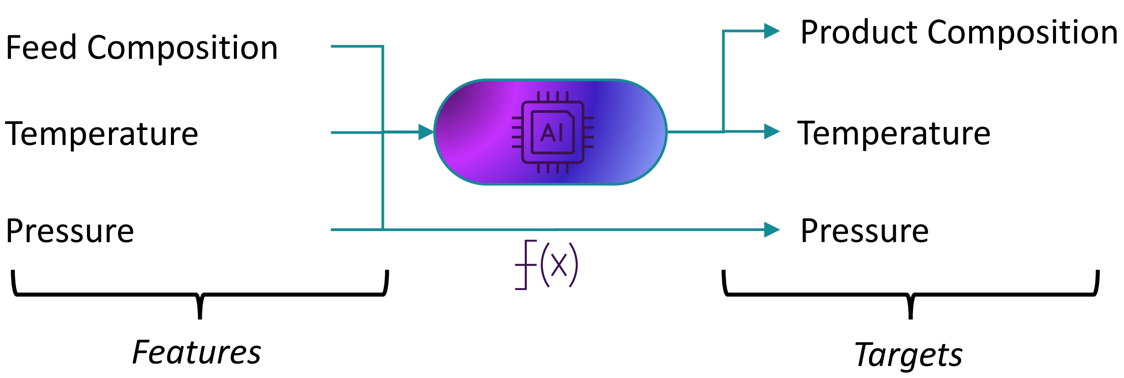
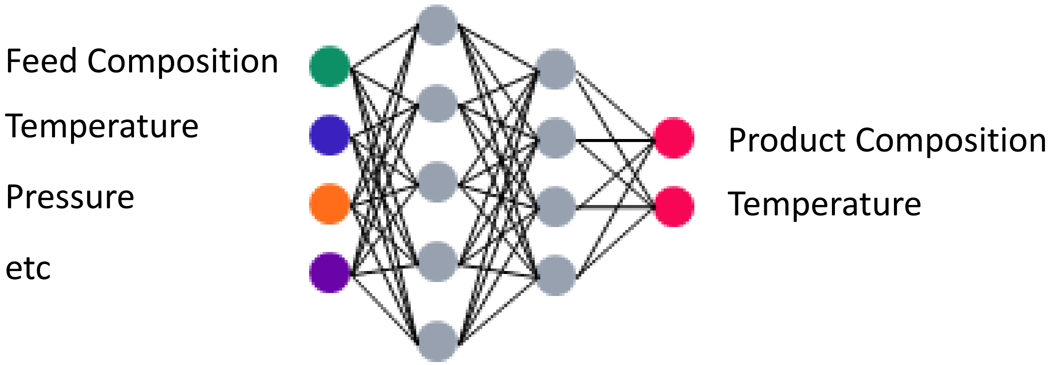
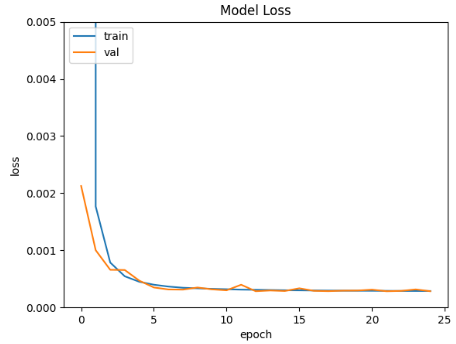
CSV





TensorFlow PyTorch scikit learn NumPy pandas matplotlib



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AVEVA™ Process Simulation

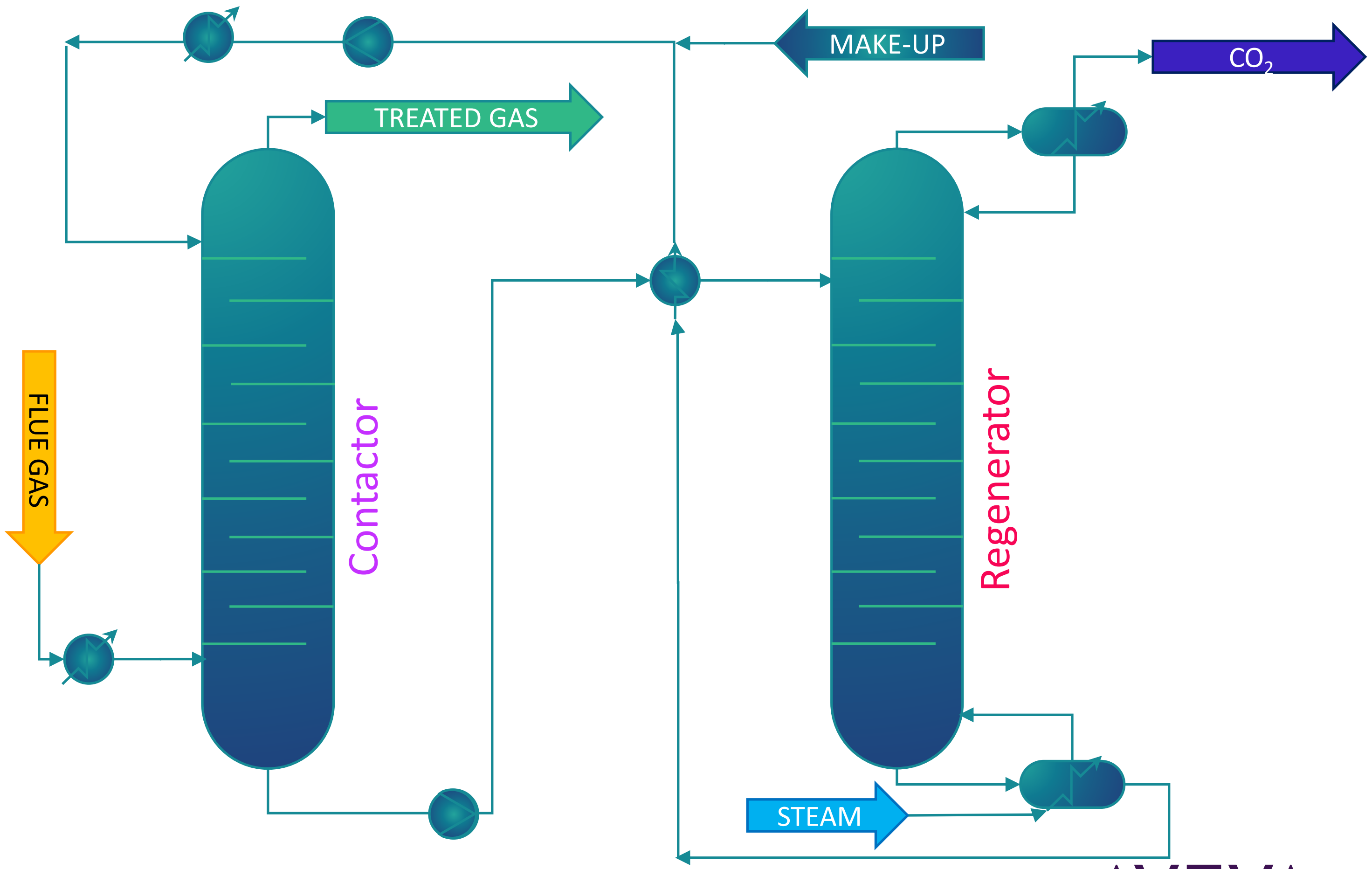
State-of-the-Art Process Simulator

- **One model for one Plant** → One APS model covers Design, Operation, Control and Asset management
- **Multiple purpose simulation** → One platform for process, utility, control, dynamic & control
- **Two way data transfer** → Two-way data transfer with AI, 3rd party coding, real time data
- **Customized & open modeling** → Easy making customized module based on 1st principle
- **Unified engineering** → Integration of simulation with PFD, P&ID 3D and engineering database

Case Study

Post Combustion Carbon Capture using Mono-Ethanol-Amine (MEA)

- Separate CO_2 from a flue gas stream coming from a combustion process
- MEA solution absorbs CO_2 in the contactor, in a regenerator the CO_2 is stripped and purified.
- Produces Treated Gas and Pure CO_2
- Energy consumption (provided by steam) is very high
- APS model is relatively complex and takes 10-20 seconds to solve
- Goal to deliver a robust and fast ML model for the CCU process that can be appended to other models generating compatible flue gas streams



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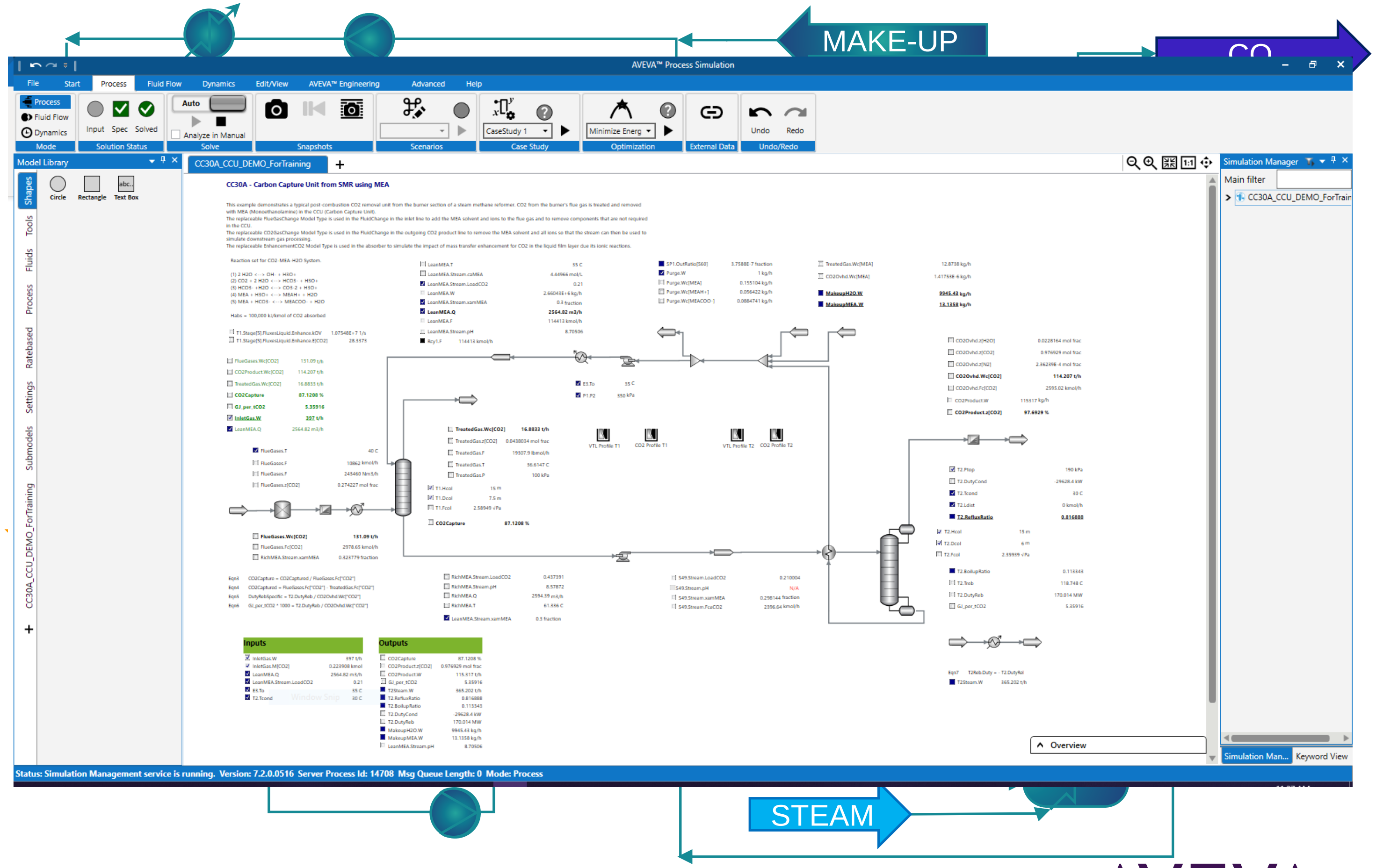
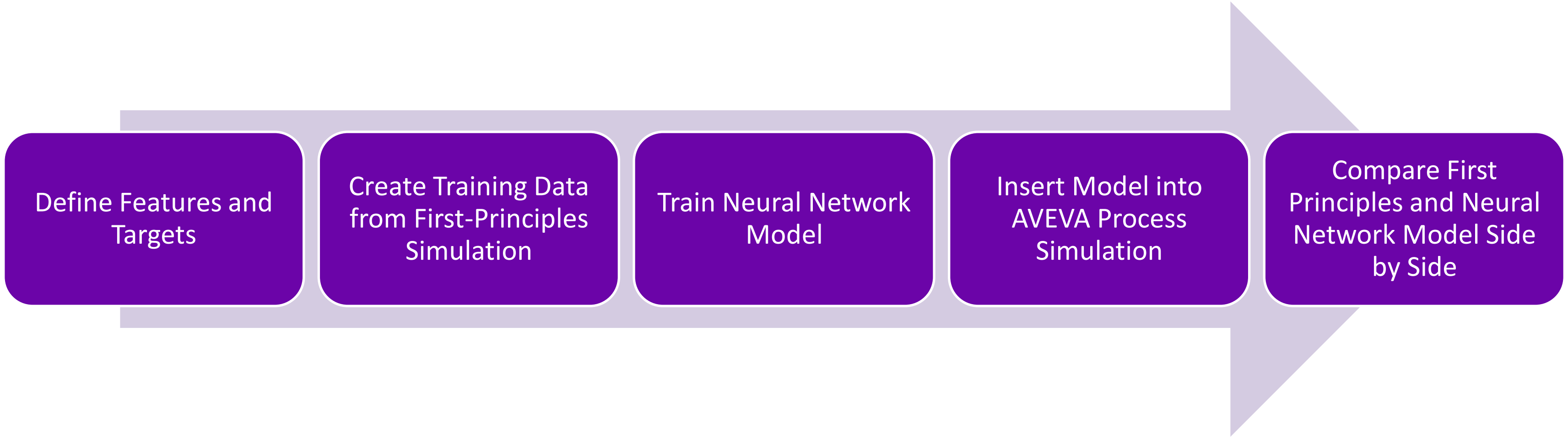


Approach



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Approach

Define Features and Targets

Create Training Data from First-Principles Simulation

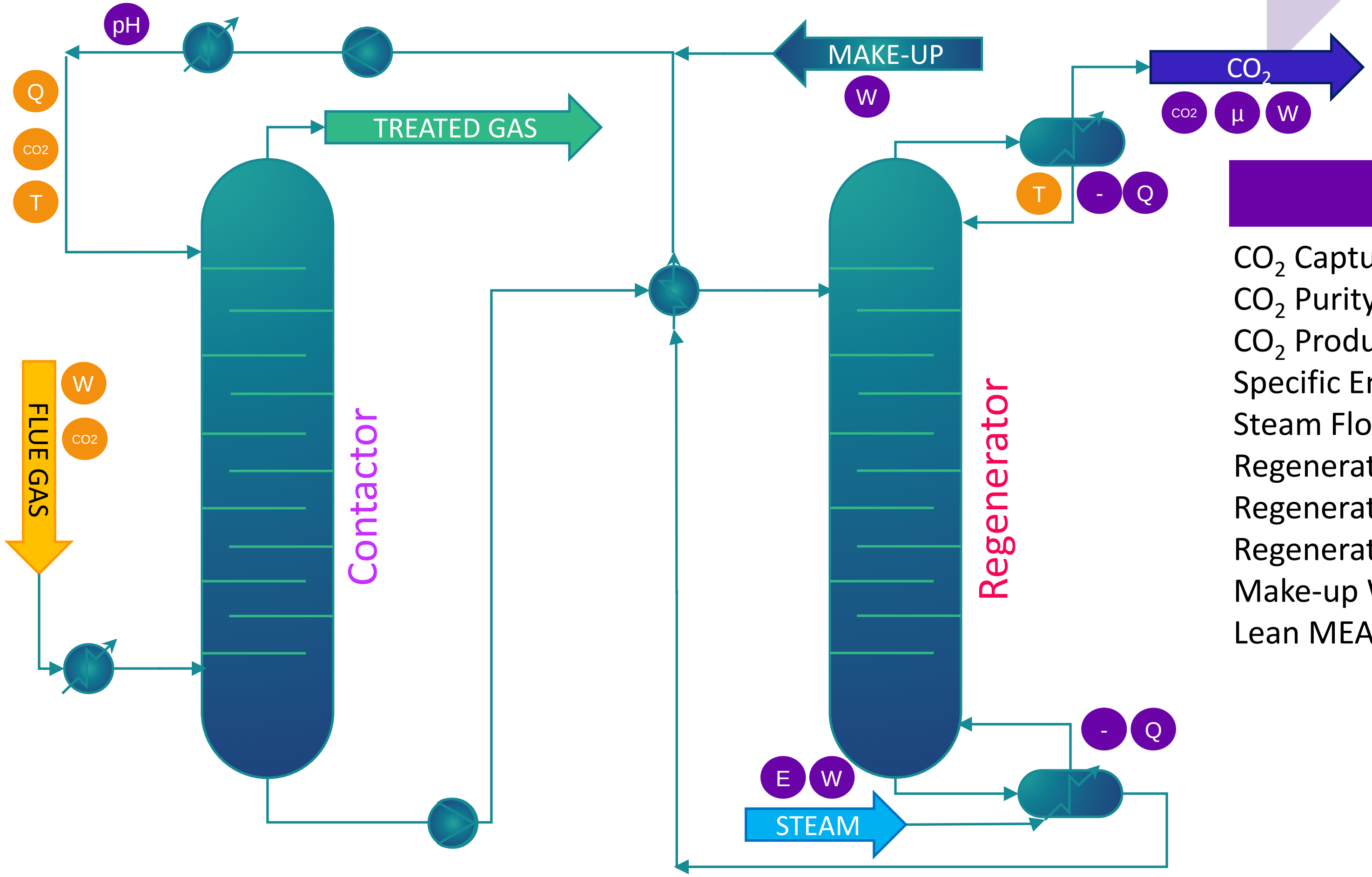
Train Neural Network Model

Insert Model into AVEVA Process Simulation

Compare First Principles and Neural Network Model Side by Side

Features

Flue Gas Mass Flow
Flue Gas CO_2 Concentration
Lean MEA Flow Rate
Lean MEA CO_2 Load
Lean MEA Temperature
Regenerator Condenser Temperature



Targets

CO_2 Capture Efficiency
CO_2 Purity
CO_2 Product Flow
Specific Energy Consumption
Steam Flow
Regenerator Reflux and Boil-up Ratios
Regenerator Condenser Duty
Regenerator Reboiler Duty
Make-up Water and MEA
Lean MEA pH

Carbonic acid

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Approach

1. Define Features and Targets
2. **Create Training Data from First-Principles Simulation**
3. Train Neural Network Model
4. Insert Model into AVEVA Process Simulation
5. Compare First Principles and Neural Network Model Side by Side

- APS scripting interface allows automated generation of training data from first principle model
- Random generation of Feature space using Latin-Hypercube sampling
- Repeat for 2000 cases

```
config_input= [
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    {"Name":    "Fluegas CO2",                       "SimName":"InletGas.M[CO2]",           "UOM":"",       "Min": 0.1,     "Max":0.25,     "Nominal":0.22398},
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    {"Name":    "Lean MEA Flow CO2 Load",            "SimName":"LeanMEA.Stream.LoadCO2",    "UOM":"",       "Min": 0.15,    "Max":0.3,      "Nominal":0.211278},
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    {"Name":    "Lean MEA T",                        "SimName":"T2.TCond",                  "UOM":"C",      "Min": 35.0,    "Max":45.0,     "Nominal":40.0},
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config_output= [
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    {"Name":    "CO2 Purity",                        "SimName":"CO2Product.z[CO2]",         "UOM":"%",         },
    {"Name":    "CO2 Mass flow rate",                "SimName":"CO2Product.W",              "UOM":"t/h",   },
    {"Name":    "Specific Energy",                   "SimName":"GJ_per_tCO2",               "UOM":"",        },
    {"Name":    "High Pressure Steam Flow rate",     "SimName":"T2Steam.W",                 "UOM":"t/h",       },
    {"Name":    "Regenerator Reflux Ratio",          "SimName":"T2.RefluxRatio",            "UOM":"",       },
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    {"Name":    "Regenerator Reboiler Duty",         "SimName":"T2.DutyReb",                "UOM":"MW",        },
    {"Name":    "Makeup Water",                      "SimName":"MakeupH2O.W",               "UOM":"kg/h",        },
    {"Name":    "Makeup MEA",                        "SimName":"MakeupMEA.W",               "UOM":"kg/h",        },
    {"Name":    "Lean MEA pH",                       "SimName":"LeanMEA.Stream.pH",         "UOM":"",       },

    ]
```

Approach

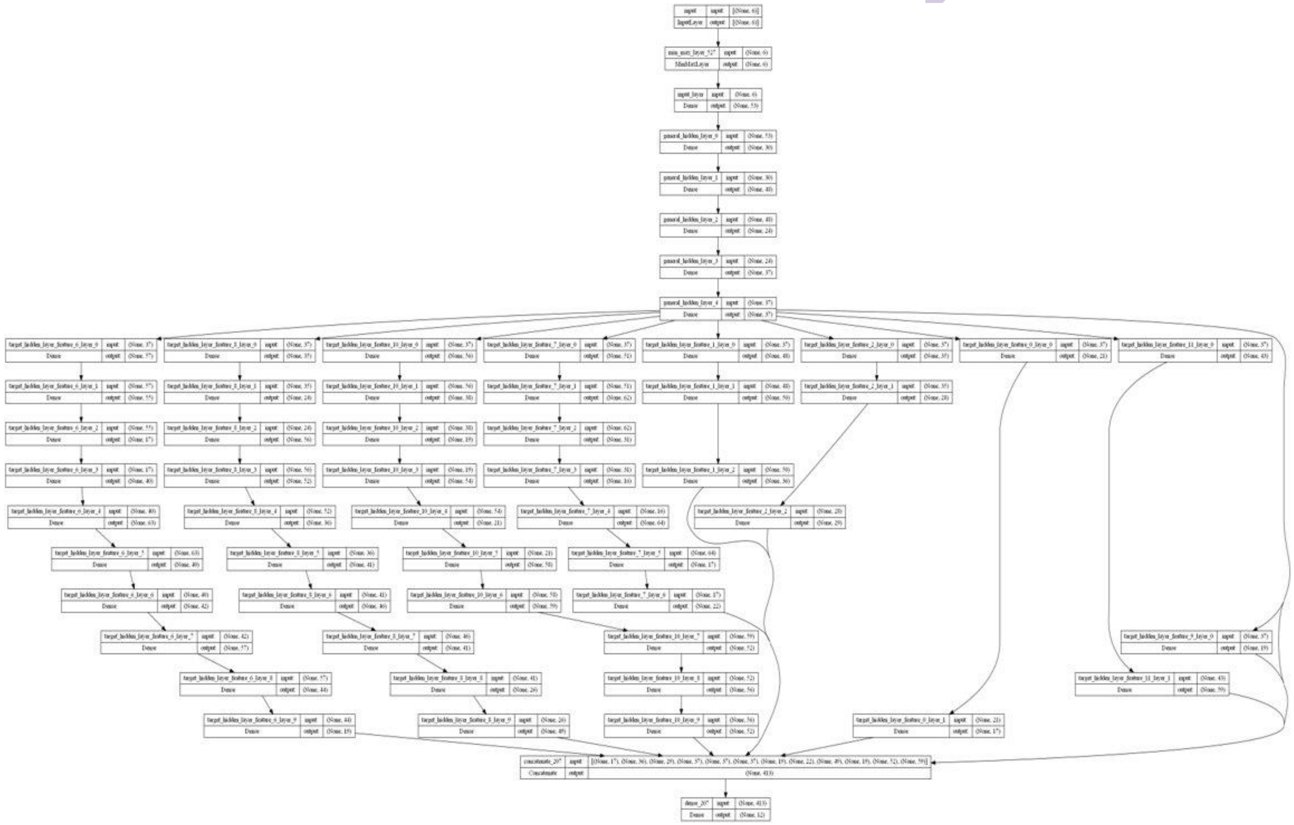
Define Features and Targets → Create Training Data from First-Principles Simulation → **Train Neural Network Model** → Insert Model into AVEVA Process Simulation → Compare First Principles and Neural Network Model Side by Side

ML Pipeline:

1. Scale features and targets

2. Optimise NN HPs and architecture

3. Train and Test



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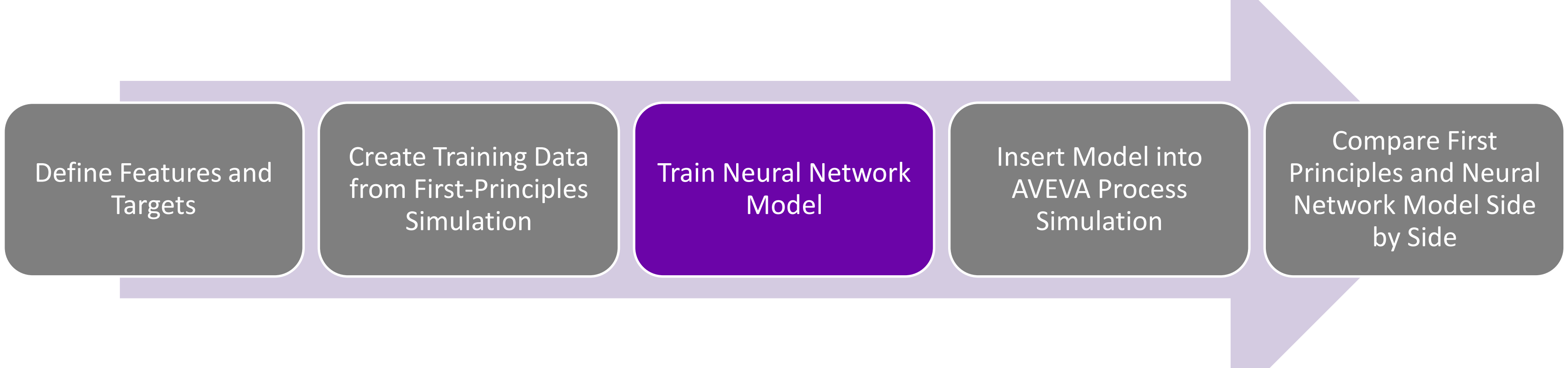
Approach



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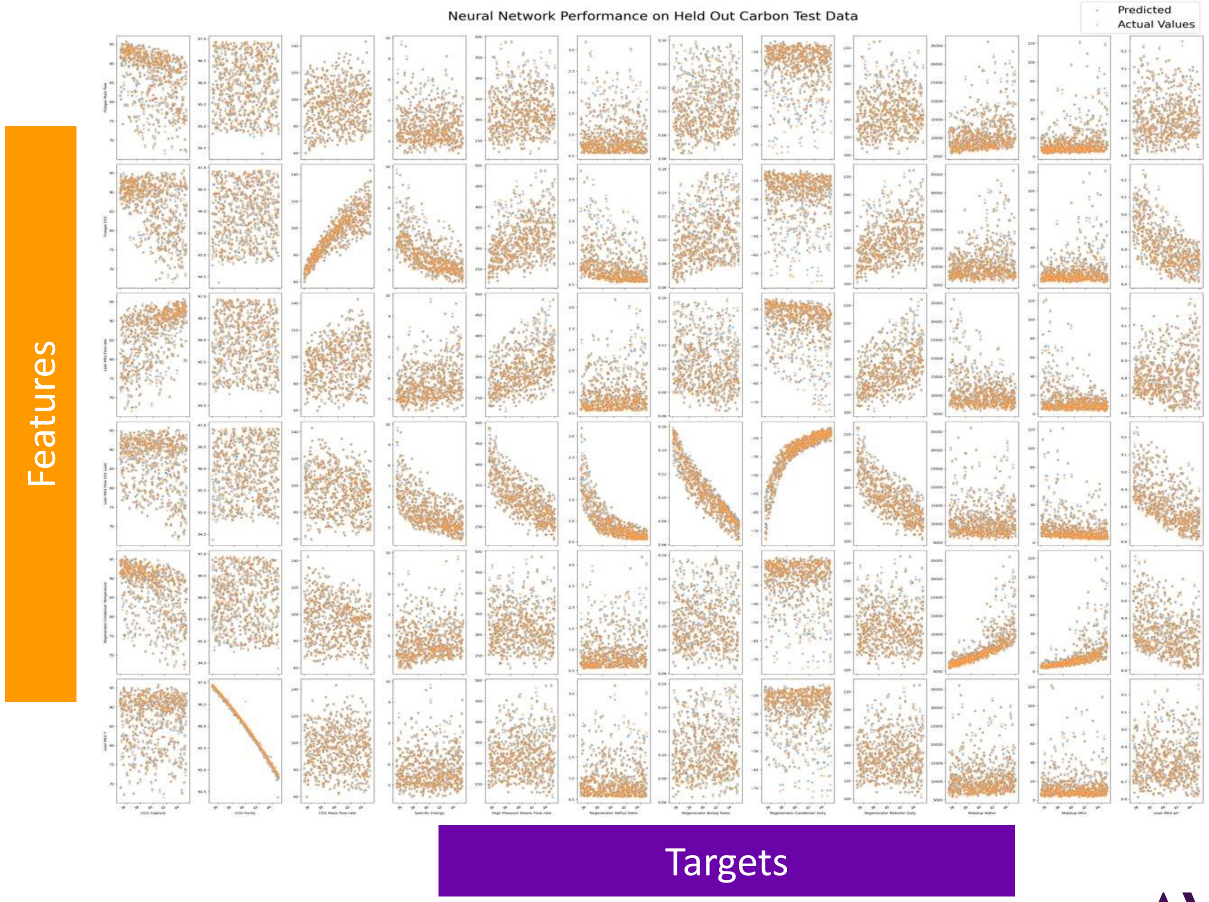

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Approach

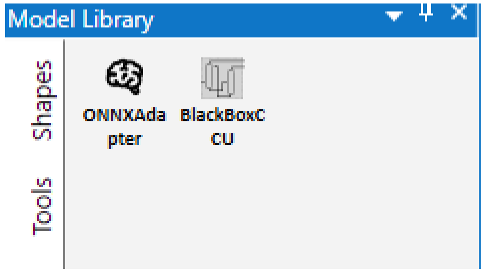
Define Features and Targets → Create Training Data from First-Principles Simulation → Train Neural Network Model → **Insert Model into AVEVA Process Simulation** → Compare First Principles and Neural Network Model Side by Side

Our Goals

- Provide a single adapter in APS to cover a wide range of externally trained models
- Do not limit ourselves to a single ML pipeline frameworks (Tensorflow, pytorch, sklearn…)
- Do not try to reimplement a whole ML runtime engine
- Make it easy for the user to drag & drop a model on the canvas, provide some configuration and let them use the model immediately

Our Approach

- Make use of ONNX (Open Neural Network eXchange)
  - Most pipelines provide a "*toONNX*" export
  - Microsoft provides open-source ONNX runtime in C#
- Encapsulate ONNX Runtime in an **External Equation Set**
- Call External Equation Set from a standard library model



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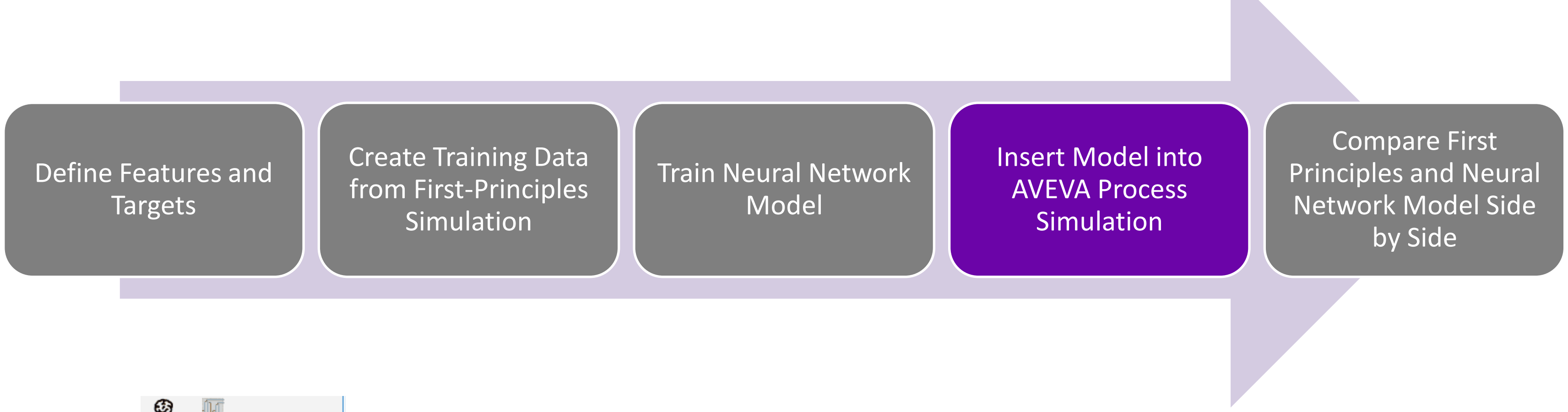
Approach



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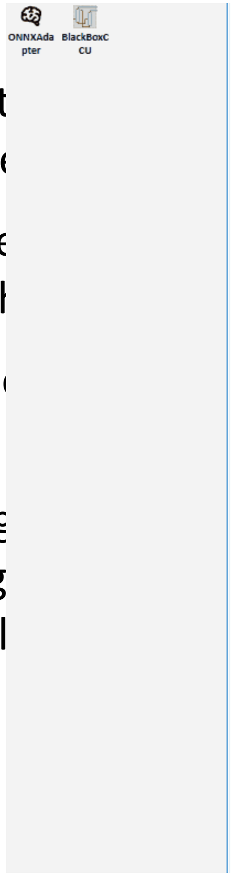


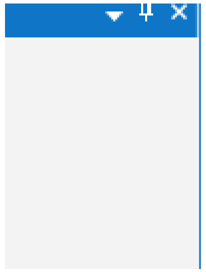
Neural Network eXchange)

toONNX" export

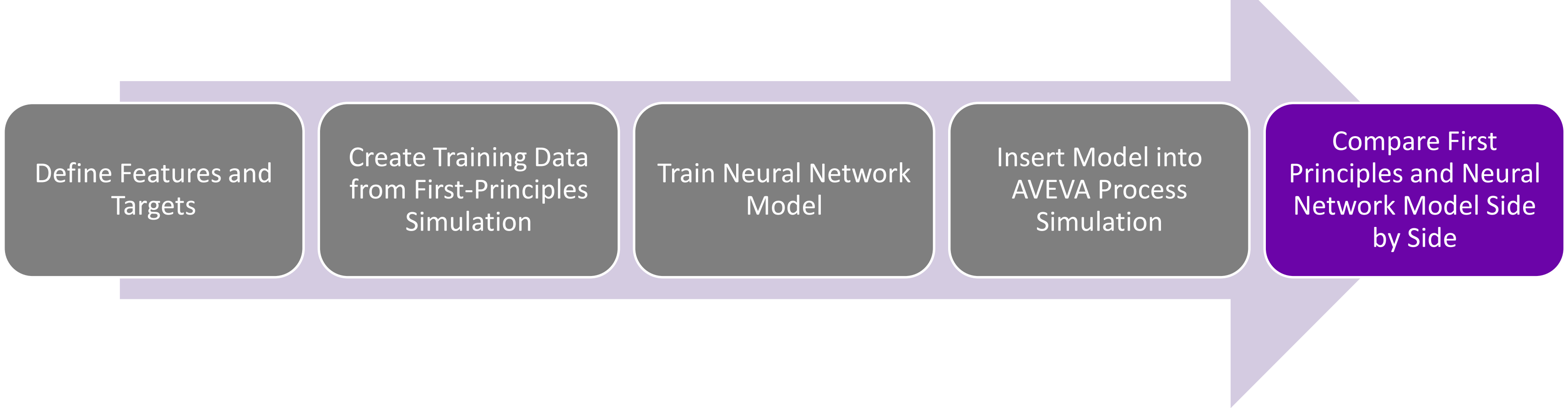
ource ONNX runtime in C#

ne in an **External Equation**

from a standard library



Approach



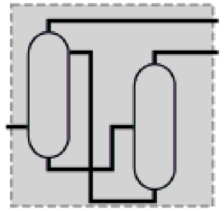
Linking Process Variables to the Black Box

InletGas.W	380 t/h	ML.Fluegas_W	380 t/h
InletGas.M[CO2]	0.223908 kmol	ML.Fluegas_M_CO2	0.223908 kmol
LeanMEA.Q	2564.82 m3/h	ML.LeanMEA_Q	2564.82 m3/h
LeanMEA.Stream.LoadCO:	0.21	ML.LeanMEA_CO2_Loading	0.21
E3.To	35 C	ML.LeanMEA_T	35 C
T2.Tcond	30 C	ML.Regenerator_T_Cond	30 C

Comparison between Real Model and Surrogate Model

CO2Capture	90.5531 %	ML.CO2_Capture	92.178 %	CO2Capture_Error	-1.79435 %
CO2Product.z[CO2]	0.976926 mol frac	ML.CO2_Purity	0.969279 mol frac	CO2Purity_Error	0.782834 %
CO2Product.W	114.728 t/h	ML.CO2_W	119.29 t/h	CO2W_Error	-3.9758 %
GJ_per_tCO2	5.37531	ML.Specific_Energy	5.21296	SpecEnergy_Error	3.02029 %
T2Steam.W	364.431 t/h	ML.High_Pressure_Steam	375.128 t/h	Steam_Error	-2.93508 %
				MAE	**2.50167 %**

Eqn1 ML.Fluegas_W = InletGas.W
Eqn2 ML.Fluegas_M_CO2 = InletGas.M[CO2]
Eqn8 ML.LeanMEA_Q = LeanMEA.Q
Eqn9 ML.LeanMEA_CO2_Loading=LeanMEA.Stream.LoadCO2
Eqn10 ML.LeanMEA_T=E3.To
Eqn11 ML.Regenerator_T_Cond=T2.Tcond



ML

Eqn12 CO2Capture_Error=(CO2Capture-ML.CO2_Capture)/CO2Capture
Eqn13 CO2Purity_Error=(CO2Product.z[CO2]-ML.CO2_Purity)/CO2Product.z[CO2]
Eqn14 CO2W_Error = (CO2Product.W-ML.CO2_W)/CO2Product.W
Eqn15 SpecEnergy_Error = (GJ_per_tCO2-ML.Specific_Energy)/GJ_per_tCO2
Eqn16 Steam_Error=(T2Steam.W-ML.High_Pressure_Steam)/T2Steam.W
Eqn17 MAE=(abs(CO2Capture_Error)+abs(CO2Purity_Error)+abs(CO2W_Error)+abs(SpecEnergy_Error)+abs(Steam_Error))/5

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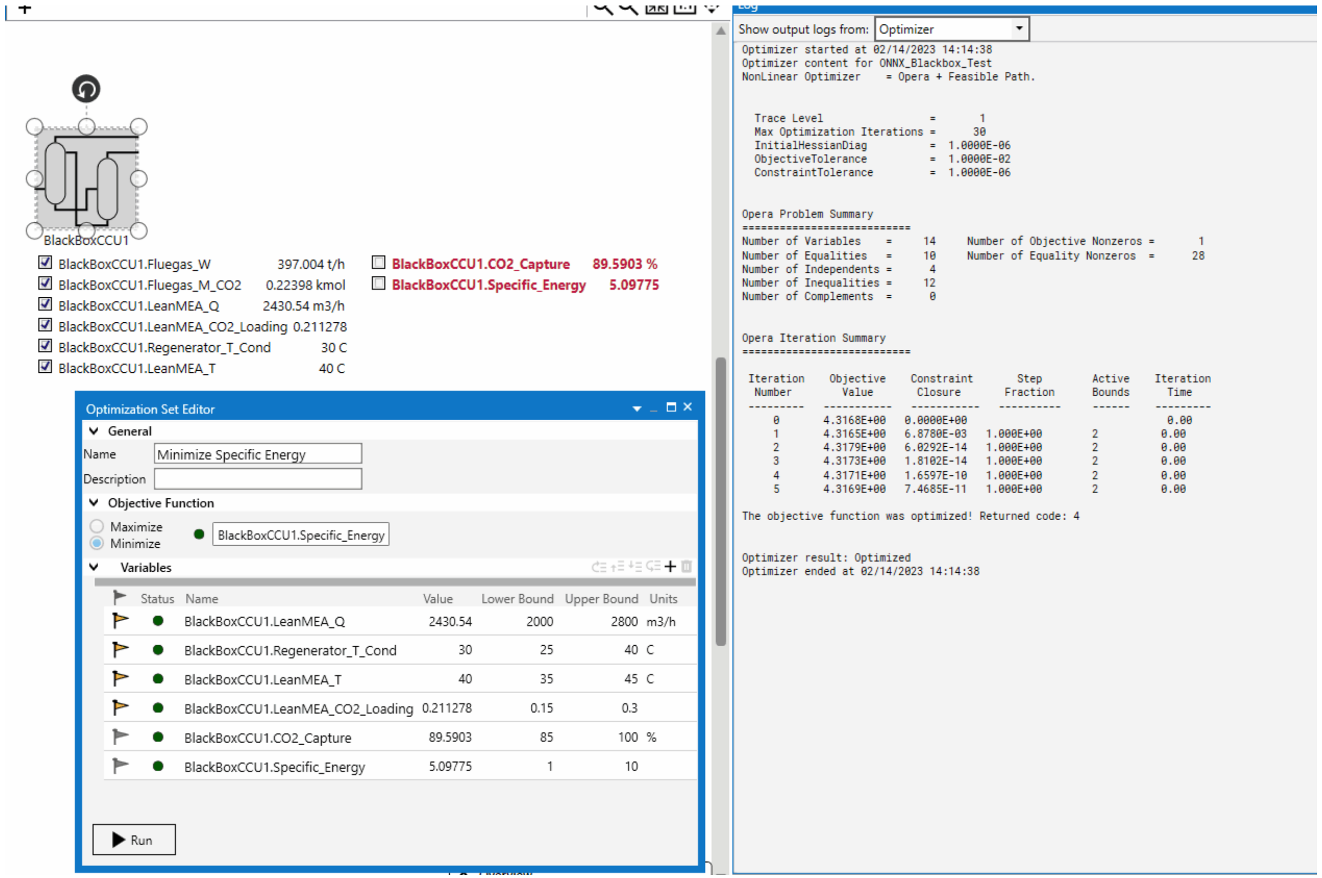

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CHEMICALS | KOREA

Isu Chemical predicts reactor yield to a 99.7% degree of accuracy

Challenge

- Optimize reactor performance and establish a catalyst replacement plan
- Building Feed & Product component structure from sample assay data

Solution

- Deployed a hybrid simulation of AVEVA™ Process Simulation and an AI reactor model to predict reactor yield and catalyst performance and decay

Results

- **Reactor yield can be predicted on different recipes and operation environments by 99.7%**
- **It is possible to predict catalyst performance and establish an efficient plan for catalyst replacement.**
- **Engineers and operators can proactively simulate the plant through an external HMI built in Excel.**

"[AVEVA Process Simulation] presents the very rigorous and powerful hybrid model combined with AI that can predict reaction yield, catalyst decay and operation performance"

DH Kim, Process Engineer, Isu Chemical

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Interview with Professor Oh

Responsible for ML model creation for ISU Chemicals Project

국립
한밭대학교

Hanbat National University, South Korea

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Takeaways

- ML models are a highly promising for modelling processes where first principles models may lack accuracy or are slow to converge
- APS now has ML platform agnostic ONNX adaptor to run ML models within the APS flowsheet and generate hybrid grey box modelling
- ISU Chemicals is an early adopter and with Hanbat University already showed success with a challenging use case for reactor performance prediction

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ABOUT AVEVA

AVEVA is a world leader in industrial software, providing engineering and operational solutions across multiple industries, including oil and gas, chemical, pharmaceutical, power and utilities, marine, renewables, and food and beverage. Our agnostic and open architecture helps organizations design, build, operate, maintain and optimize the complete lifecycle of complex industrial assets, from production plants and offshore platforms to manufactured consumer goods.

Over 20,000 enterprises in over 100 countries rely on AVEVA to help them deliver life's essentials: safe and reliable energy, food, medicines, infrastructure and more. By connecting people with trusted information and AI-enriched insights, AVEVA enables teams to engineer efficiently and optimize operations, driving growth and sustainability.

Named as one of the world's most innovative companies, AVEVA supports customers with open solutions and the expertise of more than 6,400 employees, 5,000 partners and 5,700 certified developers. The company is headquartered in Cambridge, UK.

Learn more at www.aveva.com

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