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Digital Twins for Inventory and Emissions Monitoring in the Process Industry

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Inprocess Technology and Consulting Group

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

keen to **share its knowledge** with 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

Mission

Help our clients to achieve **safer**, **greener**, more **reliable** and more **profitable** industrial operations

Emissions Challenges in the Process Industry

Issues

- Tracking internal states that cannot be measured
- Sensor solutions prohibitively expensive
- Real-time tracking virtually impossible through measurements
- Dynamic operation
- Regulators limits

It is extremely valuable to know what is internally happening with the most critical components in the process

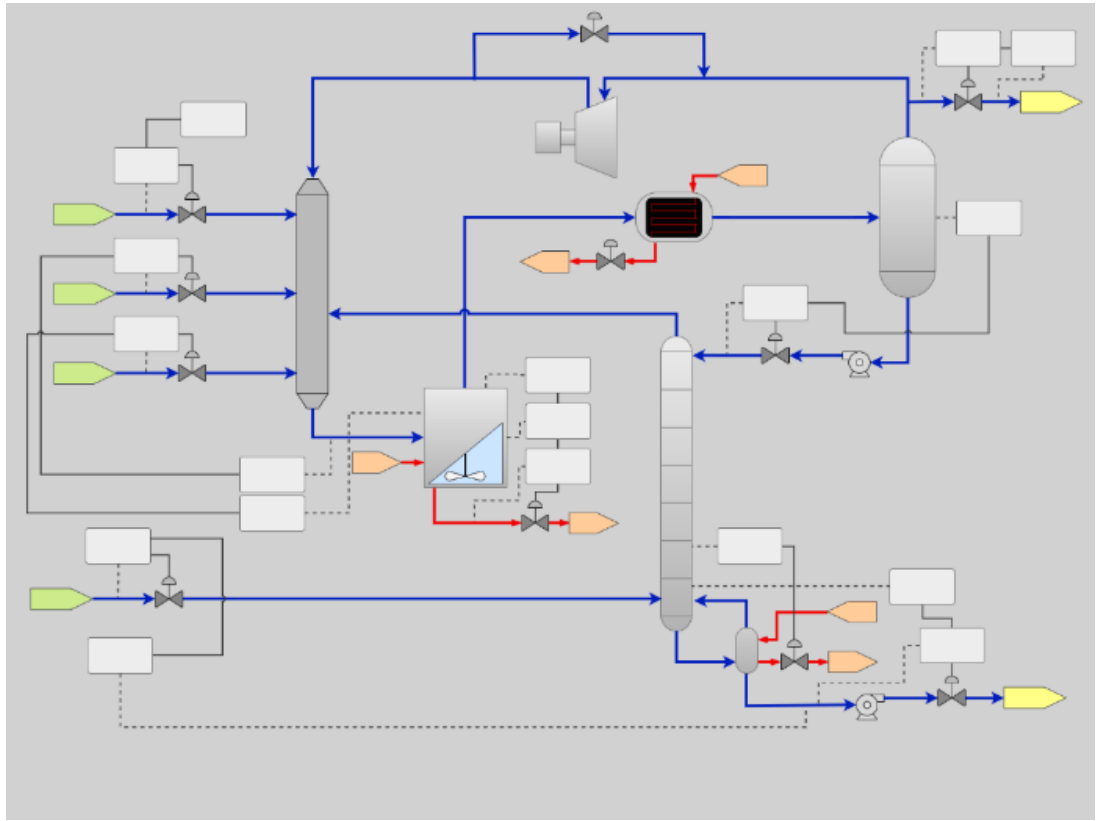
- Even if we cannot measure them directly

Let's test solutions to the monitoring issue

Emissions Challenges in the Process Industry

- **We need a case study that allows us to benchmark a new solution for this problem**
  - That accounts with enough historical data ✓
    - For normal operation AND abnormal operation
  - Simple enough to handle so that we can get insights ✓
  - Complex enough so that it is representative of the process industry dynamics ✓
  - That does not compromise client's data privacy ✓

- **We select the Tennessee Eastman Process as our reference problem**



Test Bench Process – Tennessee Eastman

Problem statement:

- Consider one of the components as a critical component
- The component is hard to track due to recycle and reactions

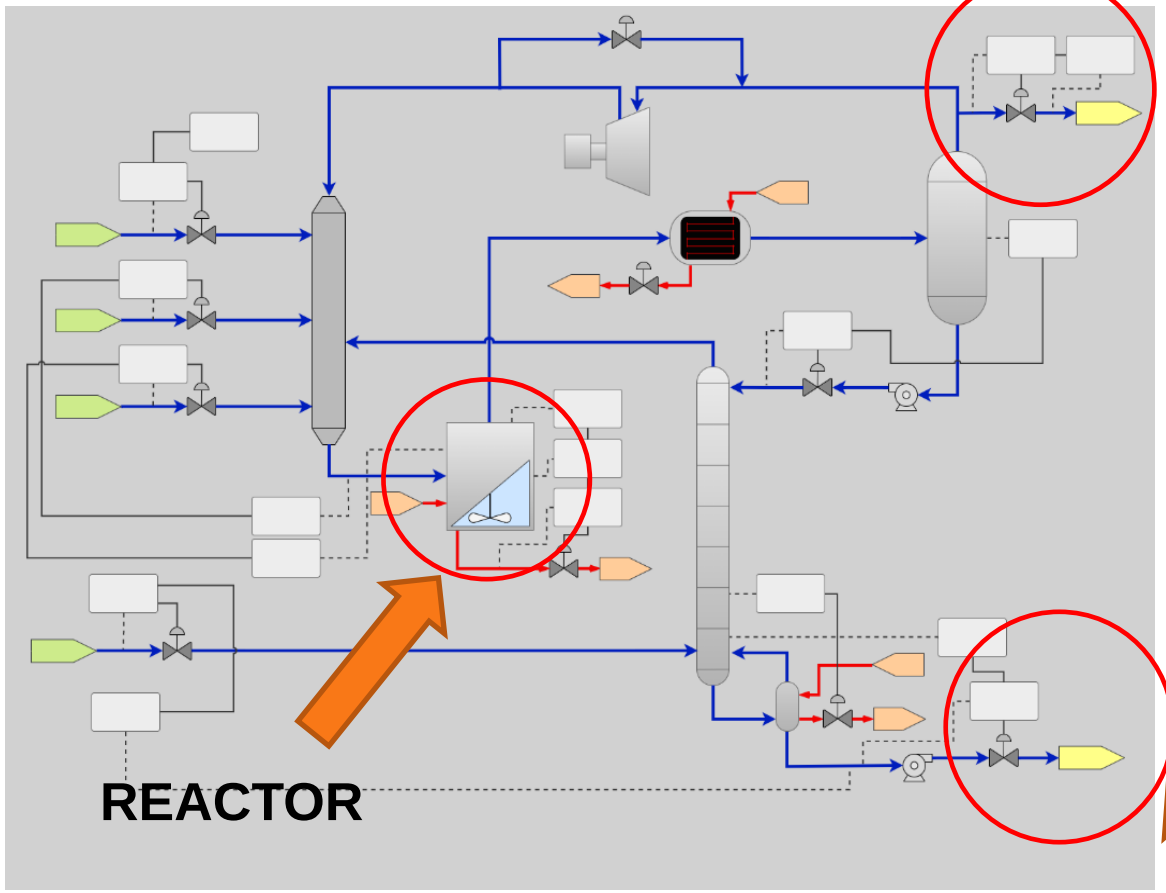
$$A + C + D \rightarrow G$$

$$A + C + E \rightarrow H$$

$$A + E \rightarrow F$$

$$3D \rightarrow 2F$$

Component	Molecular weight
A	2.0
B	25.4
C	28.0
D	32.0
E	46.0
F	48.0
G	62.0
H	76.0



Test Bench Process – Tennessee Eastman

Problem statement:

- Consider one of the components as a critical component
- The component is hard to track due to recycle and reactions
- Let's track the A inventory of this plant

$$A + C + D \rightarrow G$$

$$A + C + E \rightarrow H$$

$$A + E \rightarrow F$$

$$3D \rightarrow 2F$$

Component	Molecular weight
A	2.0
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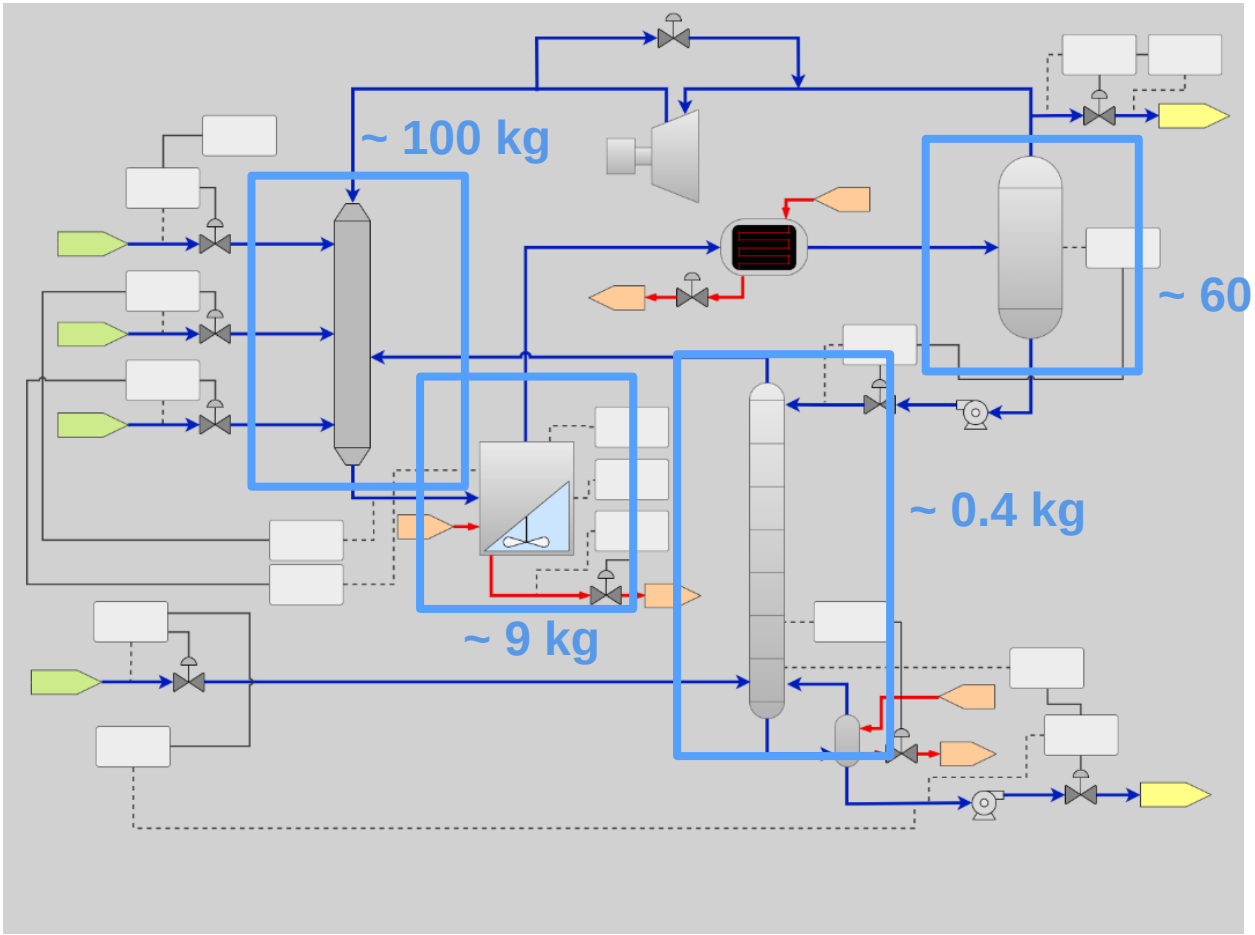
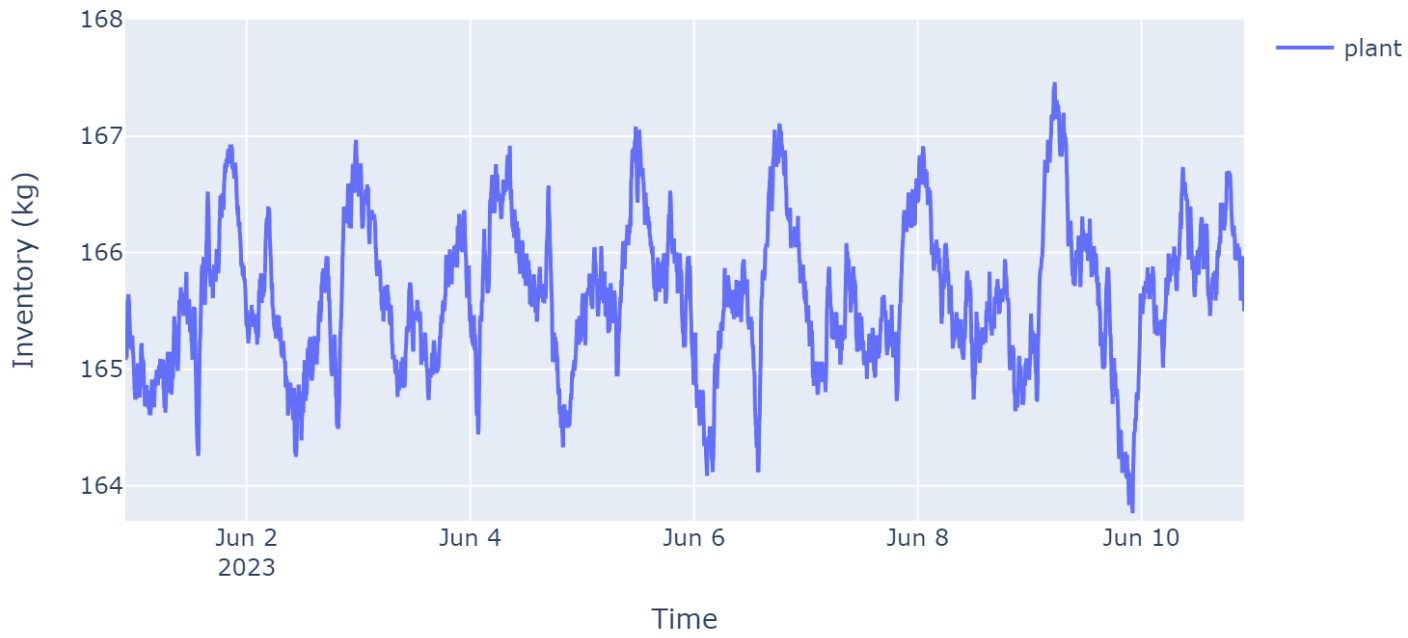


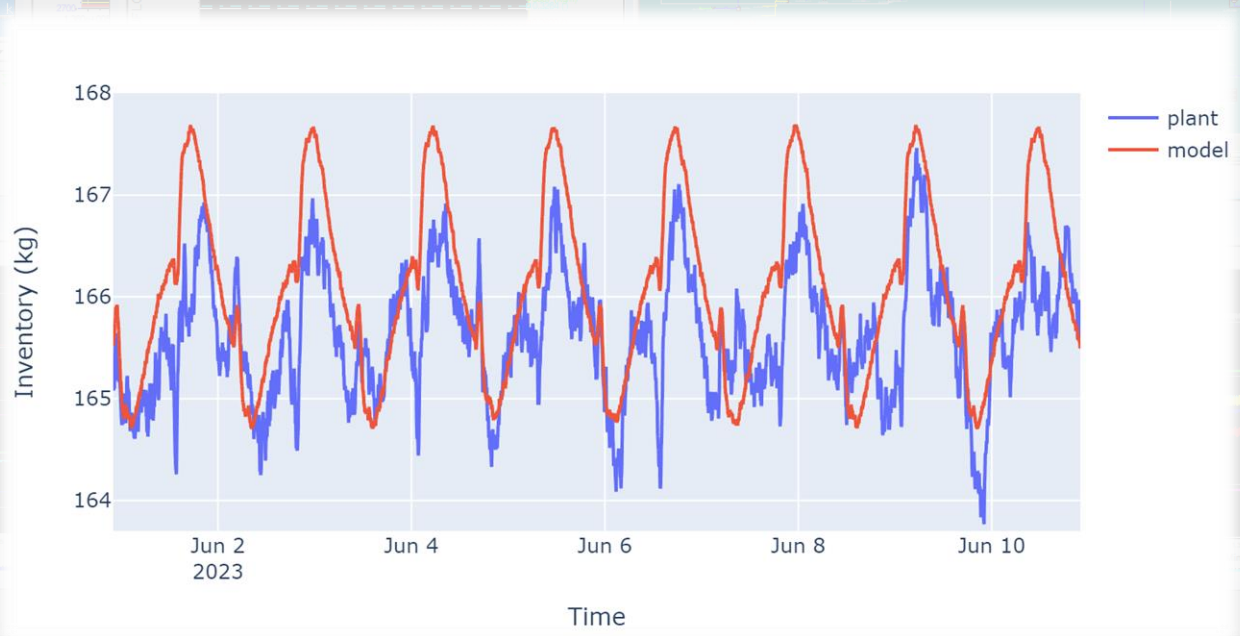
Inventory Tracking Solution

- **How can we estimate our inventories and losses? (as accurately as possible)**
  1. ~~Plant measurements~~
  2. First-principles simulation



2. First-principles Simulation

- **Dynamic replica of the asset, synchronized with real-time plant data.**
- **Tracking of the asset behavior**
- **Calculation of real-time values for temperature, pressure, flow, composition and inventories**

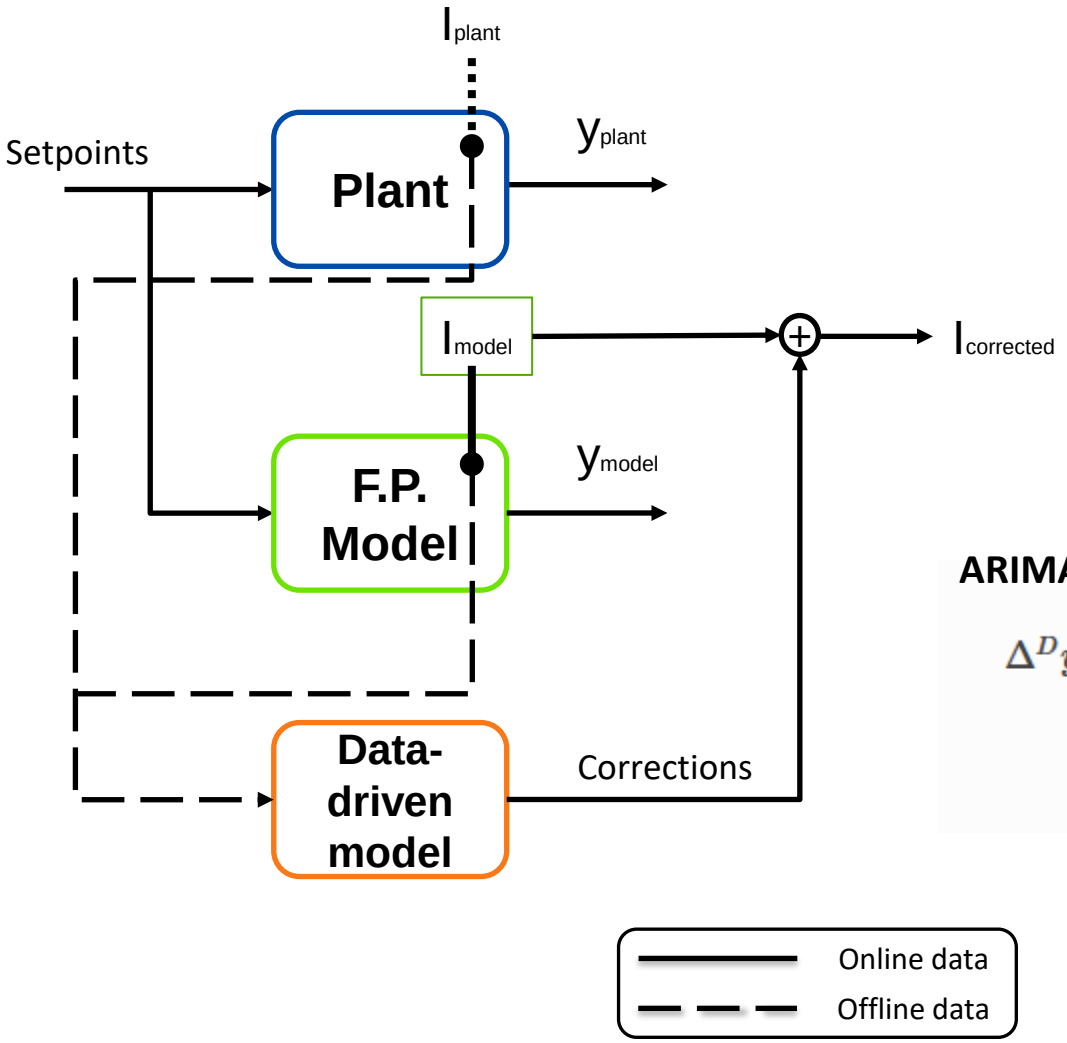


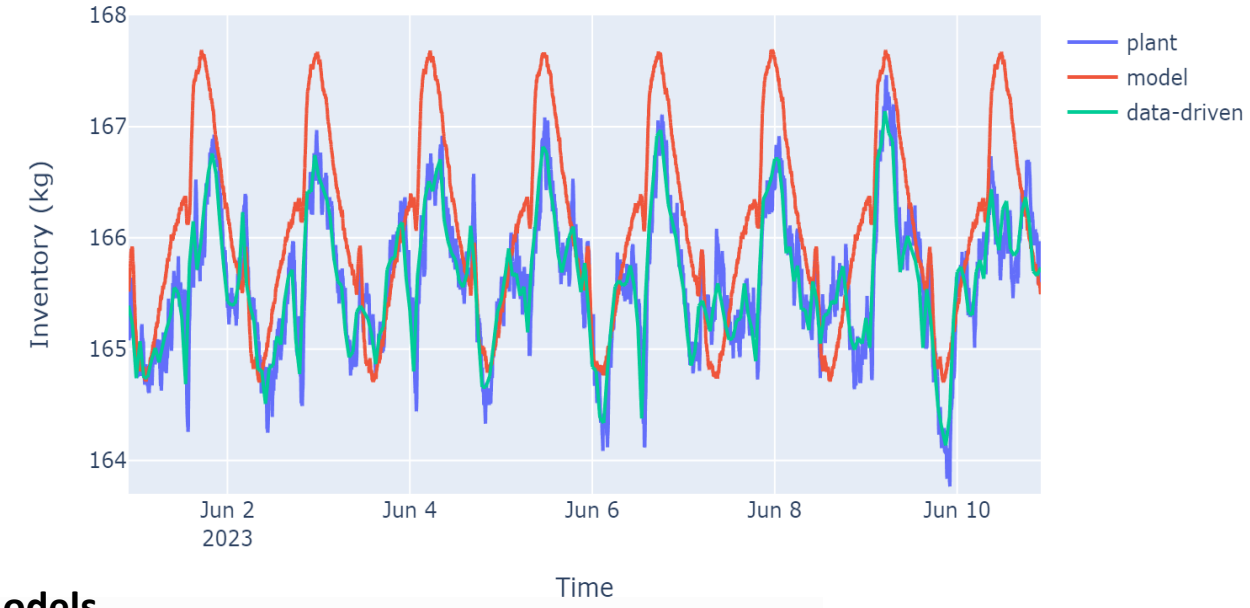
2. First-principles Simulation

- Dynamic simulation provides valuable information of the trends and state of the plant
- But it has limitation in terms of accuracy and real-time trade-off

Can we improve first-principles estimation further taking advantage of historical data?

3. Data-driven Estimate Correction



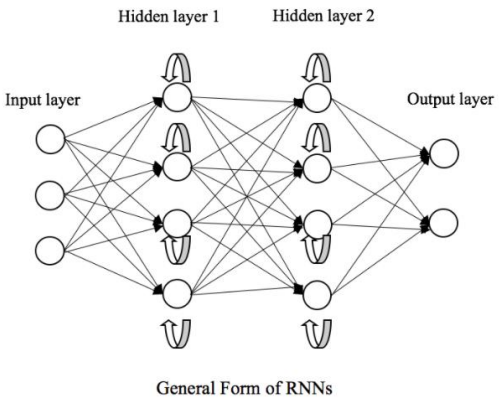


ARIMA Models

$$\Delta^D y_t = \sum_{i=1}^{p} \phi_i \Delta^D y_{t-i} + \sum_{j=1}^{q} \theta_j \epsilon_{t-j} + \sum_{m=1}^{M} \beta_m Xm, t + \epsilon_t$$

$$\epsilon_t \sim N\left(0, \sigma^2\right)$$

Recurrent Neural Networks



General Form of RNNs

3. Data-driven Estimate Correction

Advantages of data-driven correction

- Can reflect differences between first principles and the actual plant that cannot be abstracted in the model
- Easy updating upon streams of new historical data
- Are only fed by variables measured in the plant and model
- Gives good results even for abnormal conditions
- The hybrid approach reduces the time-series dynamic load on the data-driven model

Conclusion

- **Inventory and emissions monitoring is becoming more important to address economic optimization and reduce greenhouse gas emission**
- **Process simulation is one of the best tools in the market to understand and improve the behavior of your plant**
- **A data-driven layer on top of the simulation can provide a great way to target more specific goals for a digital twin and complement the model**

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