Scientific Modeling in Chemical Process Industry

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In memory of Andreas Weber (Andreas)

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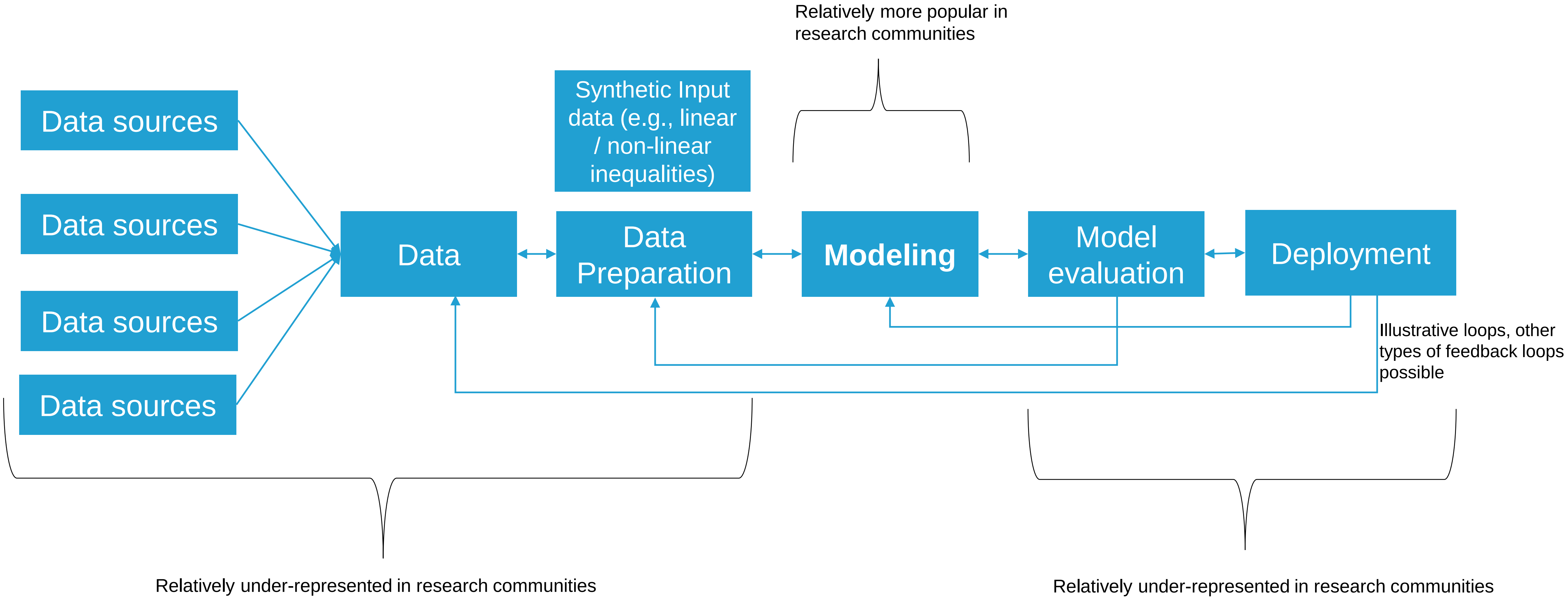
Closing Event : ANR/DFG Project SYMBIONT, Bonn, March 14-16, 2022

(My) Transition from Academia to Industry

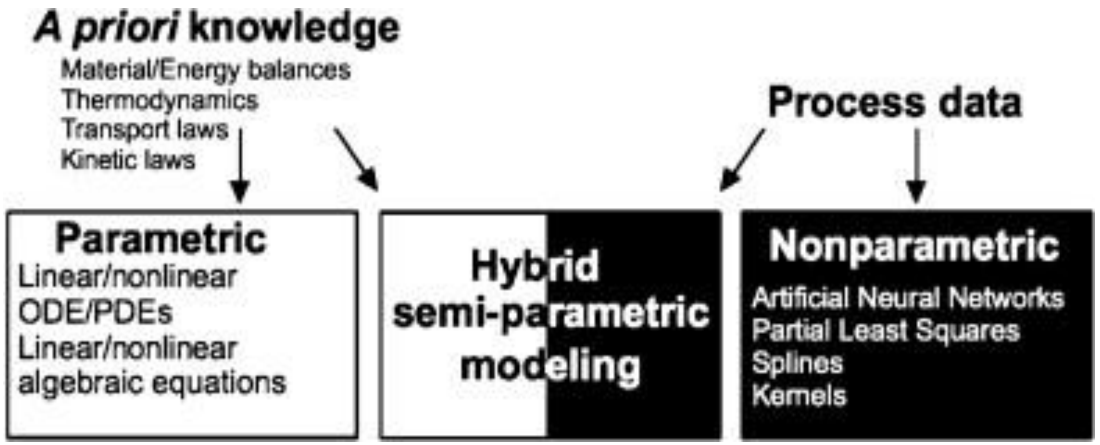
- Academia
  - Work on computational method development for a defined problem
  - Supervision of students
  - Scientific communication => publications, conferences, “open-source” code
- Industry
  - Focus on use-cases / business needs
  - Consulting with business partners, operating divisions in identifying problem statements
  - Data Preparation
  - Sync with multiple teams, management topics
  - Patents, “open-source” code possible (with careful business considerations)

Modeling Journey



We assume here that the business problem is identified and is translated to a modeling problem

Modeling
Predictive Models



Mechanistic Models / Parametric

Pros
- Extrapolation to unseen data
- Training data demand is lower
- Training data variance is lower

Cons
- Deeper process understanding
- Effort / time for model development
- Numerical simulations

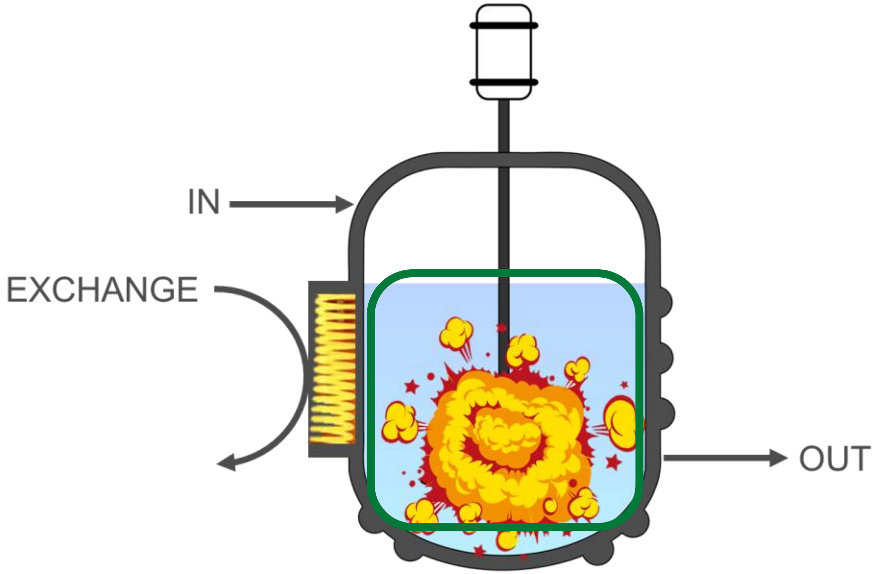
Machine Learning / Nonparametric

Pros
- Expert process understanding not required
- Time to develop the model is very short
- Inferences times are very fast

Cons
- Higher training data demand
- Higher variance in the training data to extrapolate
- Limited extrapolation

Figure adapted from von Stosch, M., Oliveira, R., Peres, J., & de Azevedo, S. F. (2014). Hybrid semi parametric modeling in process systems engineering: Past, present and future. *Computers & Chemical Engineering*, *60*, 86–101.

Mechanistic Models: The Abstraction of Reality



Assumptions and simplifications held to be true !

Process

Inputs:

$\boldsymbol{x}_0$

$\boldsymbol{u}$

State variables: $\boldsymbol{x}$

Changes in $\boldsymbol{x}$, relationship between phases and boundaries

Outputs:

$\boldsymbol{x}_f$

Balance equations, e.g., $mass, energy$

Constitutive equations, e.g., $ideal\ gas\ law$

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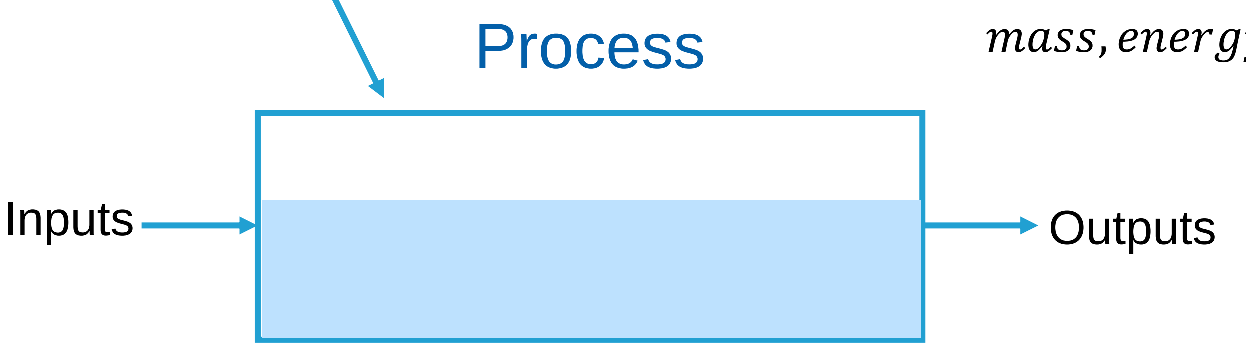
Mechanistic Models: The Equations

Assumptions:
Homogeneous!



General form of balance equation

$$\frac{d\Psi}{dt} = J_{\Psi} + J_{s,\Psi} + \Gamma_{\Psi}$$

Extensive variable, e.g., $mass, energy, momentum$ (Ψ)

Source-Sink, e.g., $Chemical\ reaction$ (Γ_{Ψ})

Convective flows, e.g., $Flows\ in\ and\ out\ of\ boundary\ volume$ (J_{Ψ})

None-convective flows, e.g., $Diffusion\ via\ boundary\ surface$ ($J_{s,\Psi}$)

Often general (integral) balance equation is formulated as:

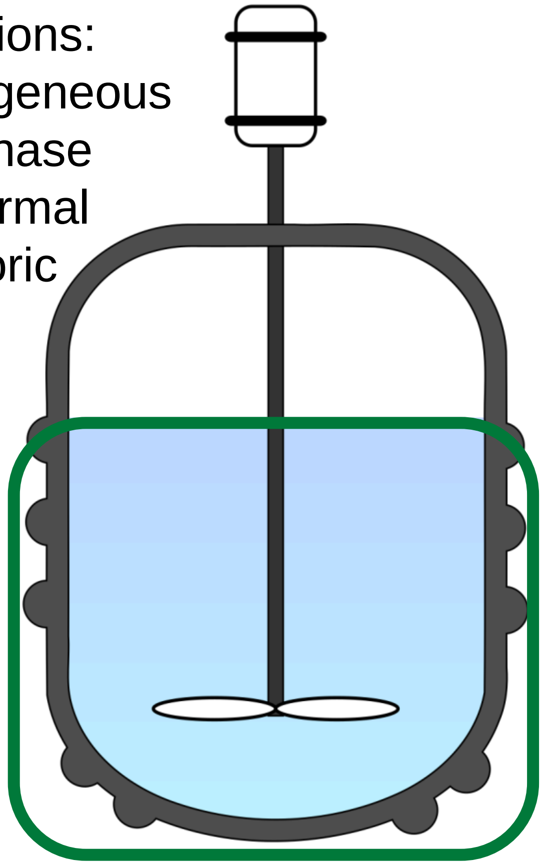
$$Accumulation = In - Out + Generation$$

Content partially adapted from Dr. Olga Walz, BASF SE

Mechanistic Models: Batch Reactor

Assumptions:

- homogeneous
- one phase
- isothermal
- isochoric



Mass balance equations: $\Psi = m_T$ or $\Psi = m_i$

batch

mass doesn't disappear

$$\frac{dm_T}{dt} = J_{m_T} + J_{s,m_T} + \Gamma_{m_T} = 0$$ conservation law $\Longrightarrow$ $m_T = \sum_{i=1}^{n_c} m_i$

homogenous, one phase

$$\frac{dm_i}{dt} = J_{m_i} + J_{s,m_i} + \Gamma_{m_i} = V_{mixture} \cdot M_{w,i} \cdot \sum_{j=1}^{n_R} \nu_{i,j} \cdot r_{i,j}$$

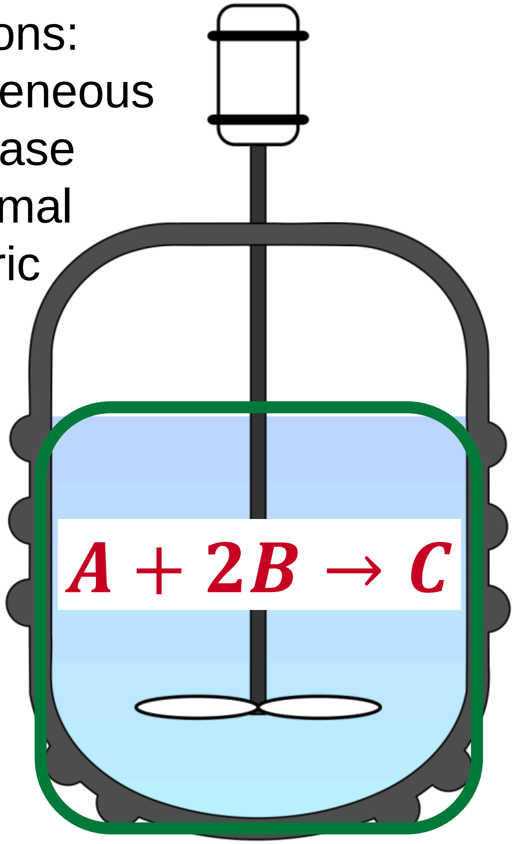
$$r_j = f\ (E_a, k_0, c_i, T), \qquad \text{e.g.,} \qquad r_j = k_{0,j} \cdot e^{\left(-\frac{E_{a,j}}{RT}\right)} \cdot \prod_{i=1}^{n_c} c_i^{p_i}$$

$$c_i = \frac{n_i}{V_{mixture}} = \frac{m_i}{V_{mixture} M_{w,i}}$$

Mechanistic Models: Batch Reactor

Assumptions:
- homogeneous
- one phase
- isothermal
- isochoric

$\nu_{1,A} = -1,$
$\nu_{1,B} = -2,$
$\nu_{1,C} = +1,$



Mass balance equations: $\Psi = m_T$ or $\Psi = m_i$

$$m_T = \sum_{i=1}^{n_c} m_i$$

$$\frac{dm_A}{dt} = V \cdot M_{w,A} \cdot -1 \cdot r_1$$

$$\frac{dm_B}{dt} = V \cdot M_{w,B} \cdot -2 \cdot r_1$$

$$\frac{dm_C}{dt} = V \cdot M_{w,C} \cdot +1 \cdot r_1$$

For a consistent model use:

(n − 1) balance equations
1 conservation equation

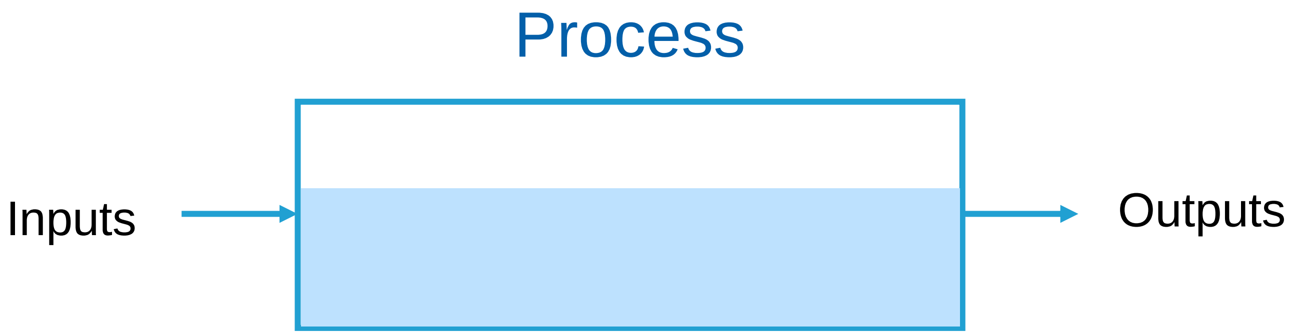
$$r_1 = k_{0,1} \cdot e^{\left(-\frac{E_{a,1}}{RT}\right)} \cdot c_A^1 \cdot c_B^{\frac{1}{3}}$$

$$c_A = \frac{n_A}{V} = \frac{m_A}{V \cdot M_{w,A}}$$

$$c_B = \frac{n_B}{V} = \frac{m_B}{V \cdot M_{w,B}}$$

$$c_C = \frac{n_C}{V} = \frac{m_C}{V \cdot M_{w,C}}$$

Data-driven Models



A typical machine learning approach

$$Ouputs = f\ (Inputs)$$

- Several existing functional forms of *f* can be used e.g., Linear regression, Neural networks, etc.
- Training: Algorithms identify the free parameters / hyper-parameters of a selected *f* based on the historical Inputs/Outputs.

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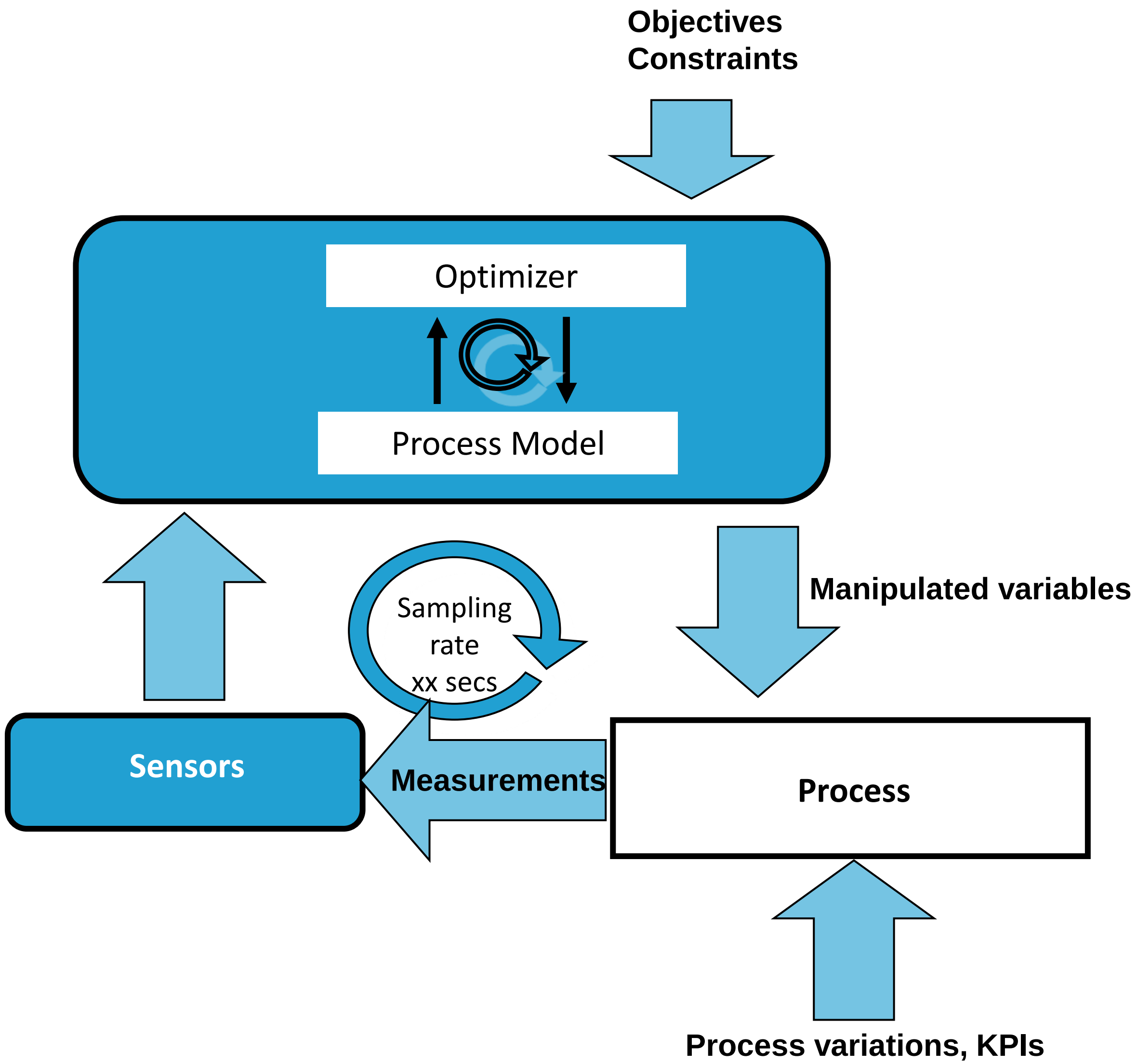
Application of Predictive Models
Process Control

- Usual tasks in machine learning include
  - Identification of the model
    - Mechanistic model
    - Data-driven model
  - Prediction i.e., evaluate the model for different (future) inputs
  - Interpretability i.e., understand the model structure and learned parameters in order to better understand the underlying process
    - Compute variable importance and sensitivities
  - Control i.e., invert the model to infer optimal inputs for desired outputs



Academic Collaboration

- Master thesis project with Prof. Dr. Holger Fröhlich, Fraunhofer SCAI, Sankt Augustin, Germany
- In 2019 TU-Berlin and BASF SE founded BASLEARN, the Berlin based Joint Lab for Machine Learning (details: https://www.baslearn.tu-berlin.de/menue/baslearn/)
- Several other collaborations exist within the area of modeling, optimization, etc..

Summary

- Several opportunities exist within BASF for application of AI / modeling solutions
  - Example: BASLEARN (w/ TU-Berlin), many more …
- More dialogue is required to align interests between Academia and Industry
  - Under-represented topics like code maintenance, IT infrastructure, data quality, robust model evaluations, underlying mathematics, etc.
- Successful AI solutions often requires a range of skills (consulting, software development, modeling ,etc.)
  - Partly mitigated by interdisciplinary teams
- Personally, an exciting journey so far…

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Professional Career

- Bachelor of Technology in Bioinformatics (Noida, India), MSc Life Science Informatics (Bonn, Germany)
- PhD in AG Prof. Dr. Andreas Weber and Prof. Dr. Holger Fröhlich (Bonn, Germany), 2016
  - Symbolic methods (Tropical Geometry)
  - Computational Systems Biology
  - Cross-exchange with other disciplines (e.g., Mathematics, Non-linear Dynamics, Biology, etc)
- Post-doc in the AG Prof. Dr. Andreas Schuppert (RWTH Aachen, Germany), 2019
  - Hybrid modeling topics
  - Focus on modeling of clinical data (Intensive Care Units)
  - Symbolic methods (“Symbiont” project)
- Production Artificial Intelligence, BASF SE, current position
  - Internal use cases with focus on machine learning / hybrid modeling topics
  - Method development
  - Industry - Academic collaboration (BASLEARN, BASF/TU-Berlin initiative)