PURDUE UNIVERSITY

Systems Engineering and Process Safety

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Research Group

Fundamental Research	Applications	People and projects
Mathematical Optimization under Uncertainty	Energy systems optimization, chemical process design and operation, supply chain	Asha: Distributed manufacturing of the electrified processes Kaiyu: Integrated scheduling and control Casper: Electrification of Process Heating (co-advised with Dr. Cornelius Masuku)
Machine Learning	Fault detection, speech/image recognition, computational biology, Acceleration of optimization algorithms	Chi: end-to-end learning of optimization problems Hao: Explainable ML for fault detection Yen-Chun: ML for stem cell (co-advised with Dr. Xiaoping Bao)

Mathematical Programming under Uncertainty

Deterministic Optimization Model

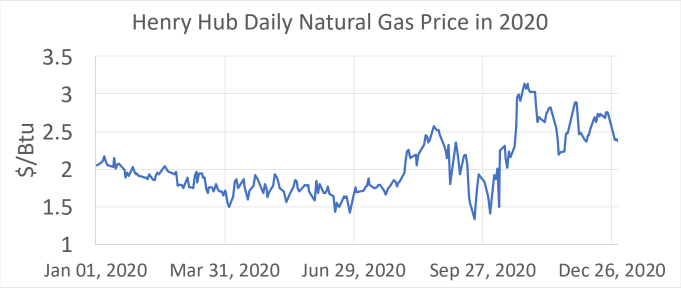
- Model **decision-making** process as an **optimization** problem

$$
\begin{aligned}
\min \quad & f(x, y, \theta) \\
s.t. \quad & g(x, y, \theta) \leq 0 \\
& h(x, y, \theta) = 0 \\
& x \in X, y \in Y
\end{aligned}
$$

- **Variables** continuous x, discrete y the capacity of process (x), whether to install a process or not (y)
- **Constraints** g, h the mass balance, to satisfy the customer demand
- **Objective** f minimize total cost
- **Parameters** θ Product demand, unit cost, thermal and kinetic properties
- The input parameters θ can be uncertain.

Sources of Parameter Uncertainty

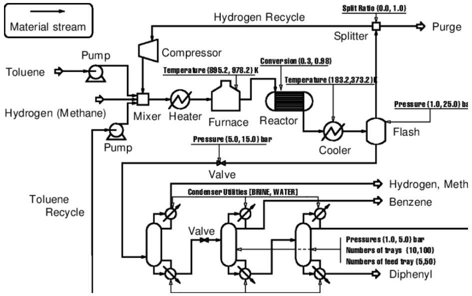
- Long-term forecasts, e.g., natural gas price



- Short-term changing conditions, e.g., extreme weather



- Real-time inaccurate measurement, e.g., temperature, pressure



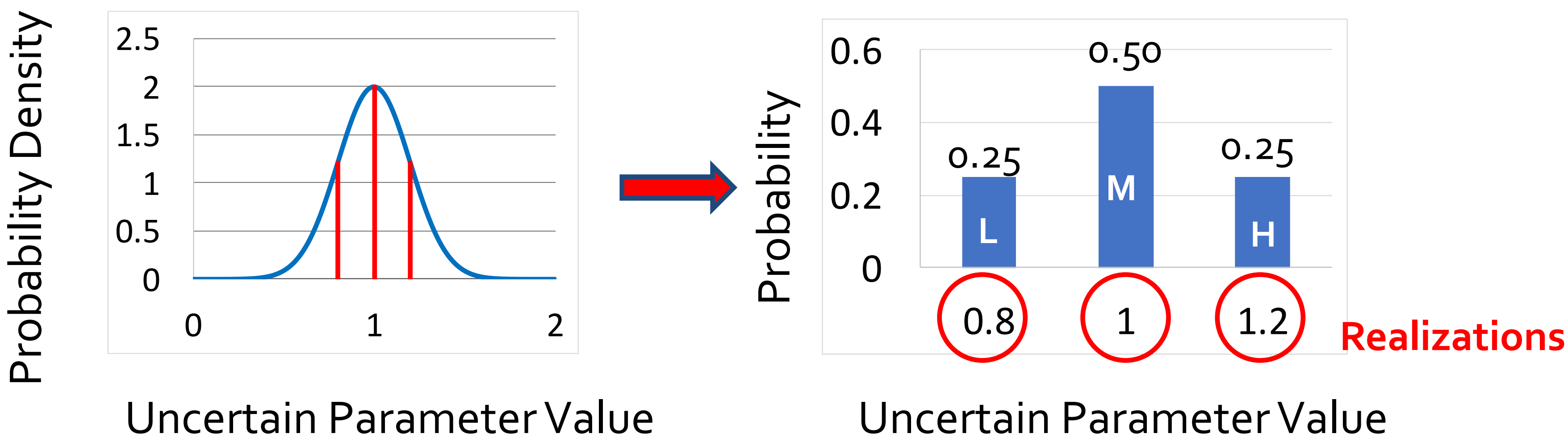
How Do We Model Uncertainty in Optimization Problems?

- Not a uniquely-defined problem
  - **Multiple** ways to hedge against uncertainty

The jungle of stochastic optimization
(credit: Warren Powell)

Stochastic Programming

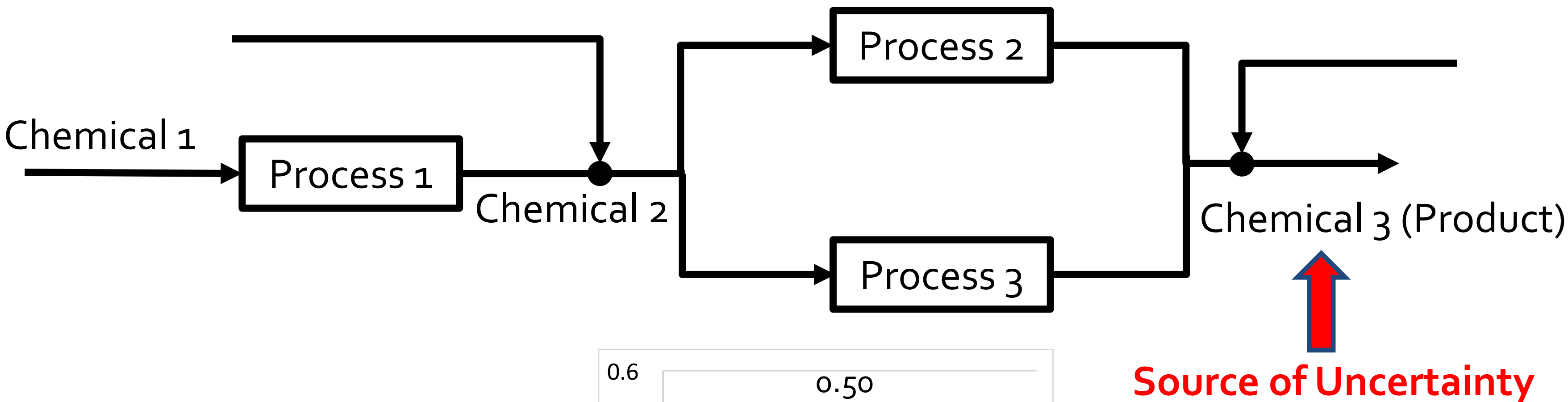
- **Stochastic programming** is a framework for modeling optimization problems that involve uncertainty (Birge and Louveaux, 2011)
- Uncertainty can be characterized by **probability distributions** known *a priori*
  - Continuous distributions → Discrete distributions

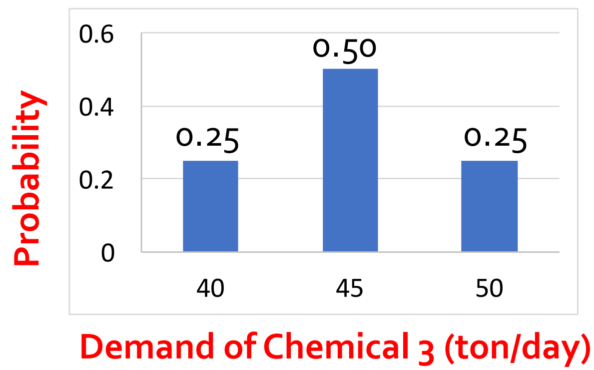


- Each realization of uncertainty parameters is called **a scenario**
- Optimize the **expected value** of the objective over all possible scenarios, i.e., **a risk-neutral approach**
- Common framework: **Two stage stochastic programming**

A Motivating Example

- **Superstructure**



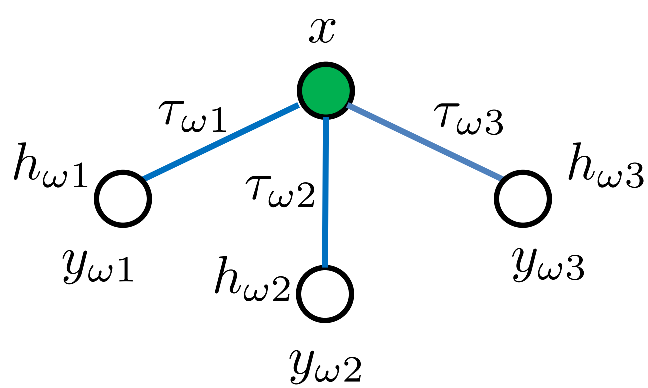


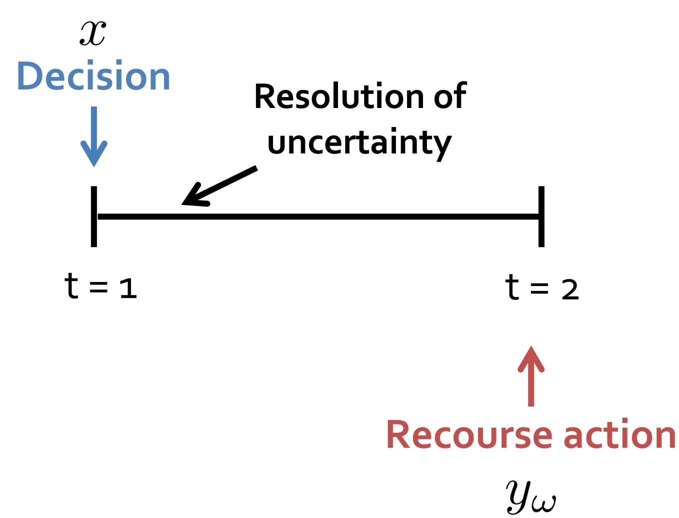
- **First stage decisions:** which process to install, the capacity of each process
- **Second stage decisions:** the mass flow rate of each stream
- **Constraints:** satisfy customer demands, mass balance

Two Stage Stochastic Programming

- First stage decisions: **Here and now**
- Second stage decisions: **Wait and see, Recourse decisions**

$$
\begin{aligned}
\min \quad & c^T x + \sum_{\omega \in \Omega} \tau_\omega d_\omega^T y_\omega \\
s.t. \quad & Ax \leq b \\
& W_\omega y_\omega \leq h_\omega - T_\omega x \qquad \forall \omega \in \Omega \\
& x \in \{x = (x1, x2) : x_1 \in \{0,1\}^n, x_2 \geq 0\} \\
& y_\omega \in \{y : y \geq 0\}
\end{aligned}
$$

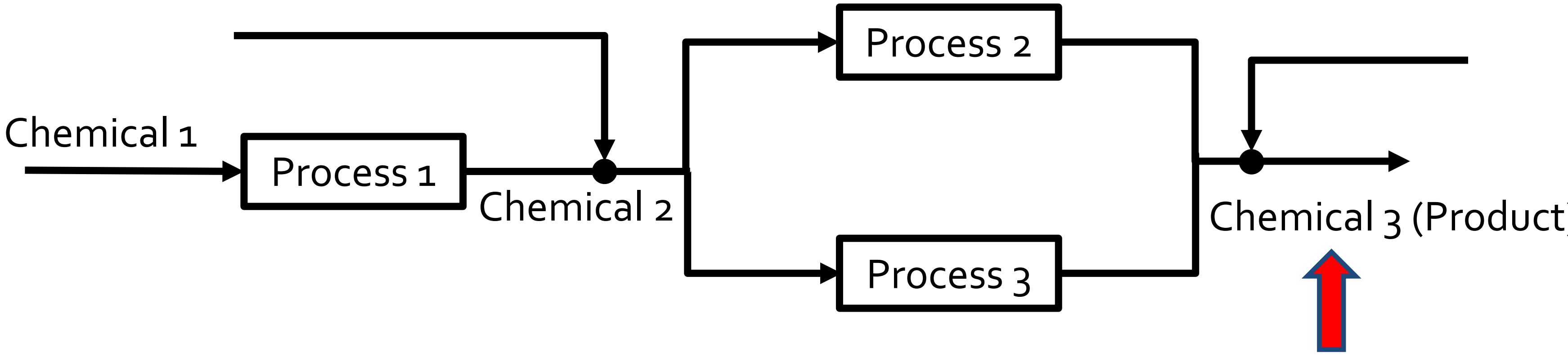




Deterministic Equivalent

Investment Planning of Process Networks

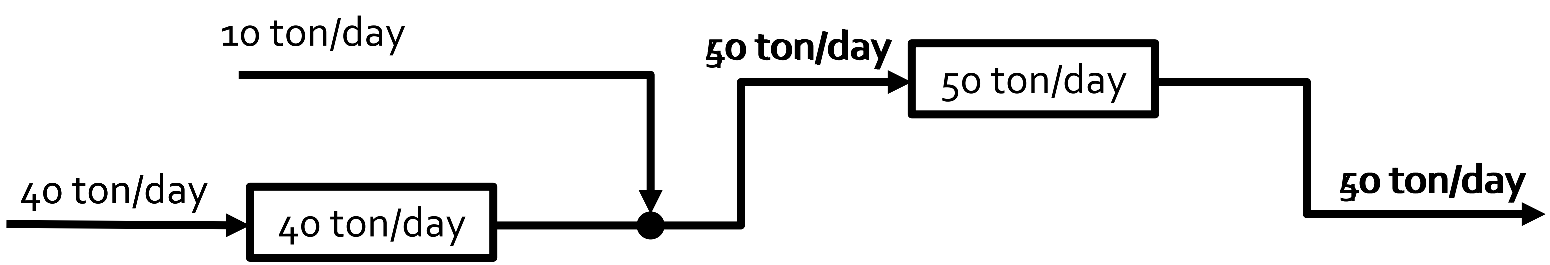
- **Superstructure**



Source of Uncertainty

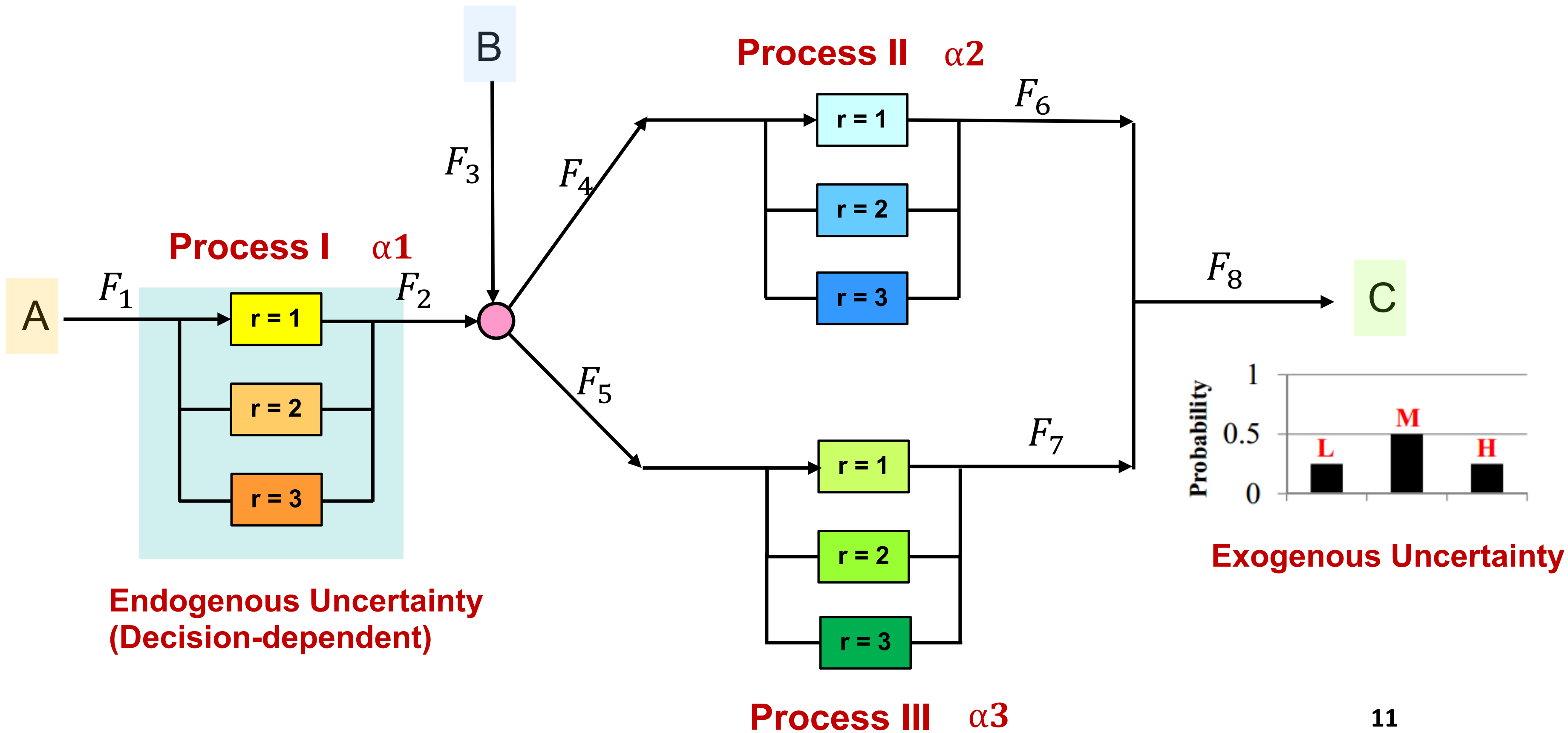
- **First stage decisions**
- **Second stage decisions**

High demand
Low demand



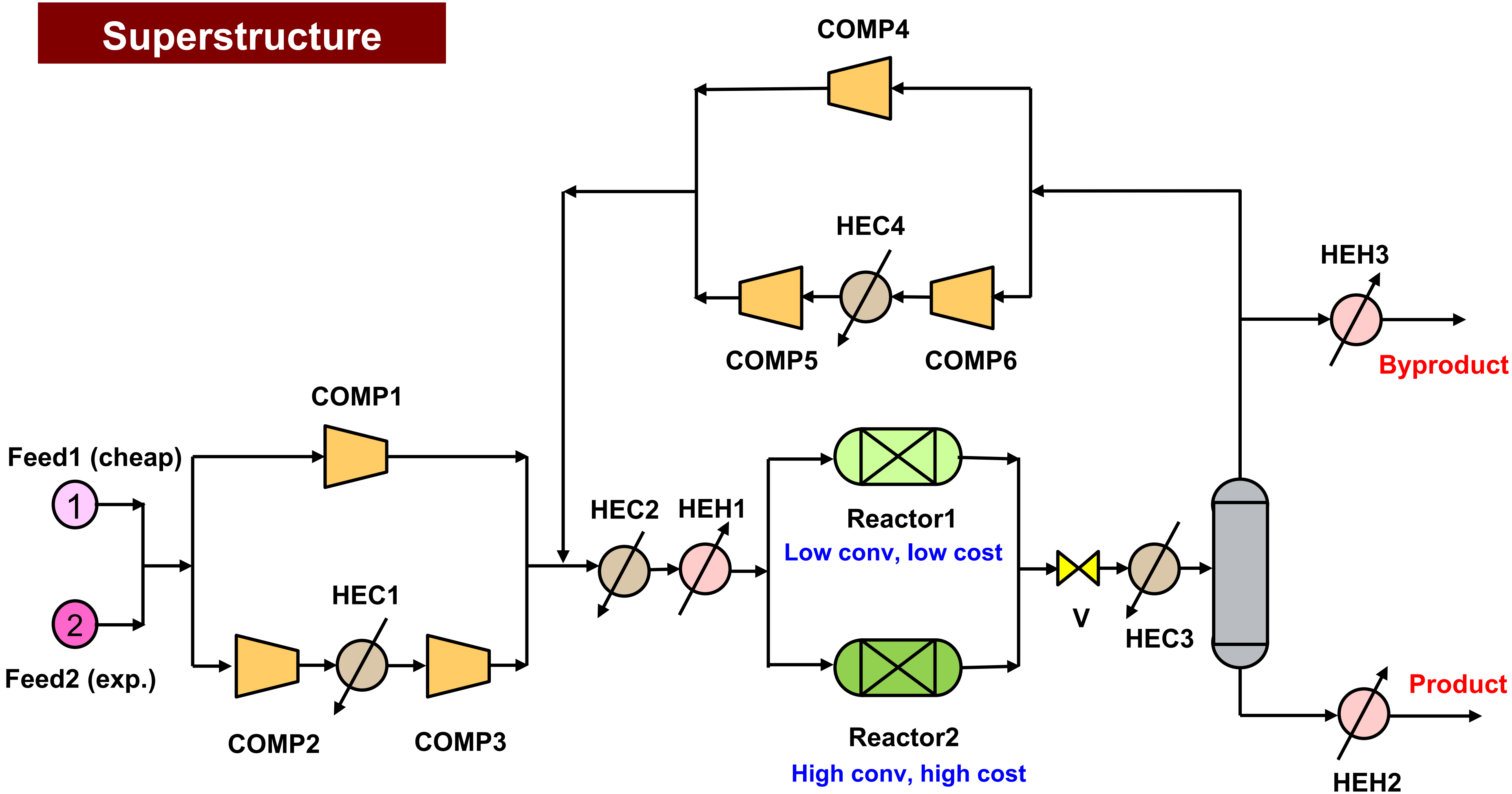
Extension to Process Reliability

- Motivation: Process units may fail
- Solution: Have backup units to improve reliability
- Trade-off: Investment cost v.s. system reliability



Industrial Methanol Synthesis

Superstructure

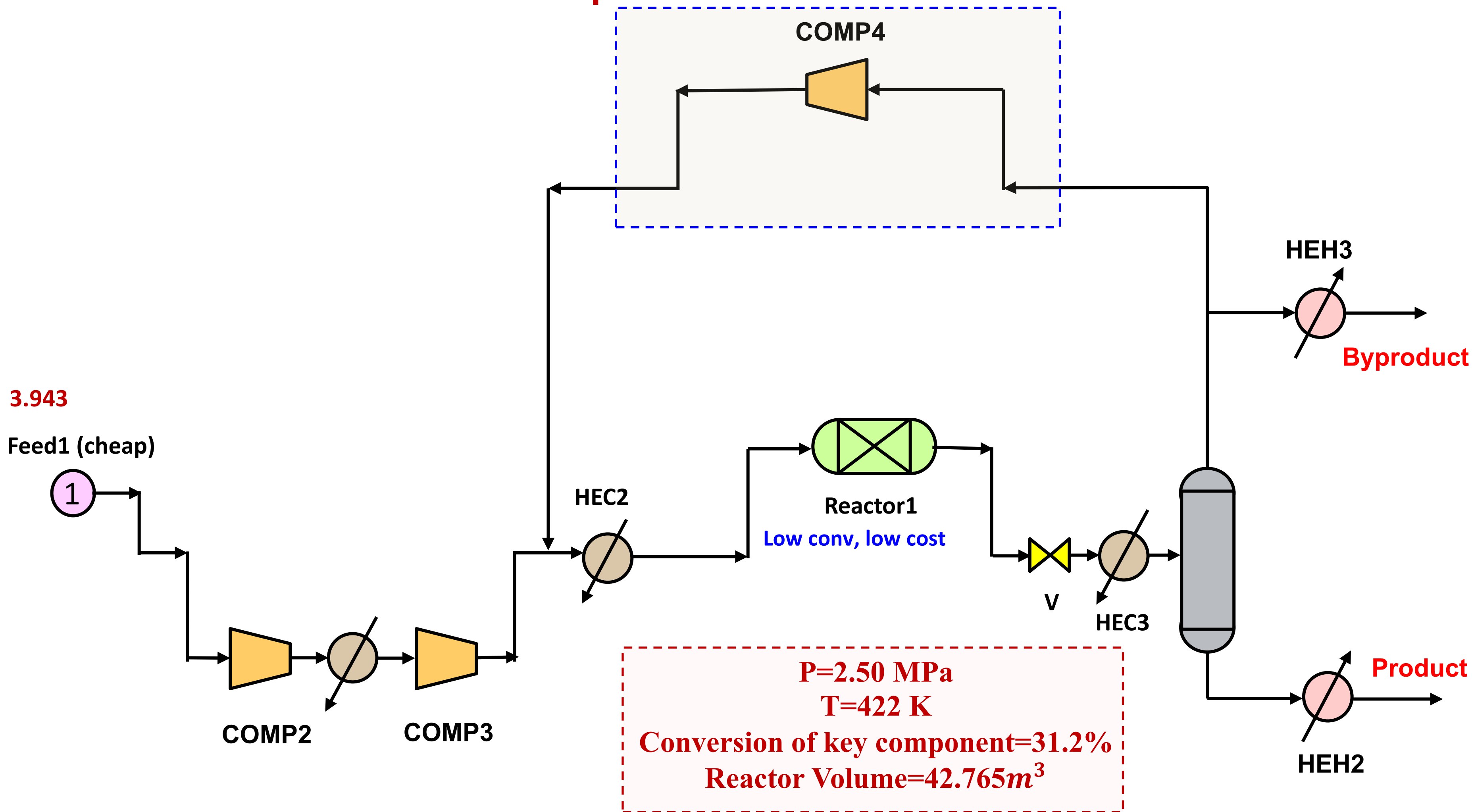


Key optimization variables in the reactors:
operating pressure and the conversion per pass

Industrial Methanol Synthesis

Deterministic Model

Profit = 4115.3749 ($1000 PER YEAR)
Too optimistic

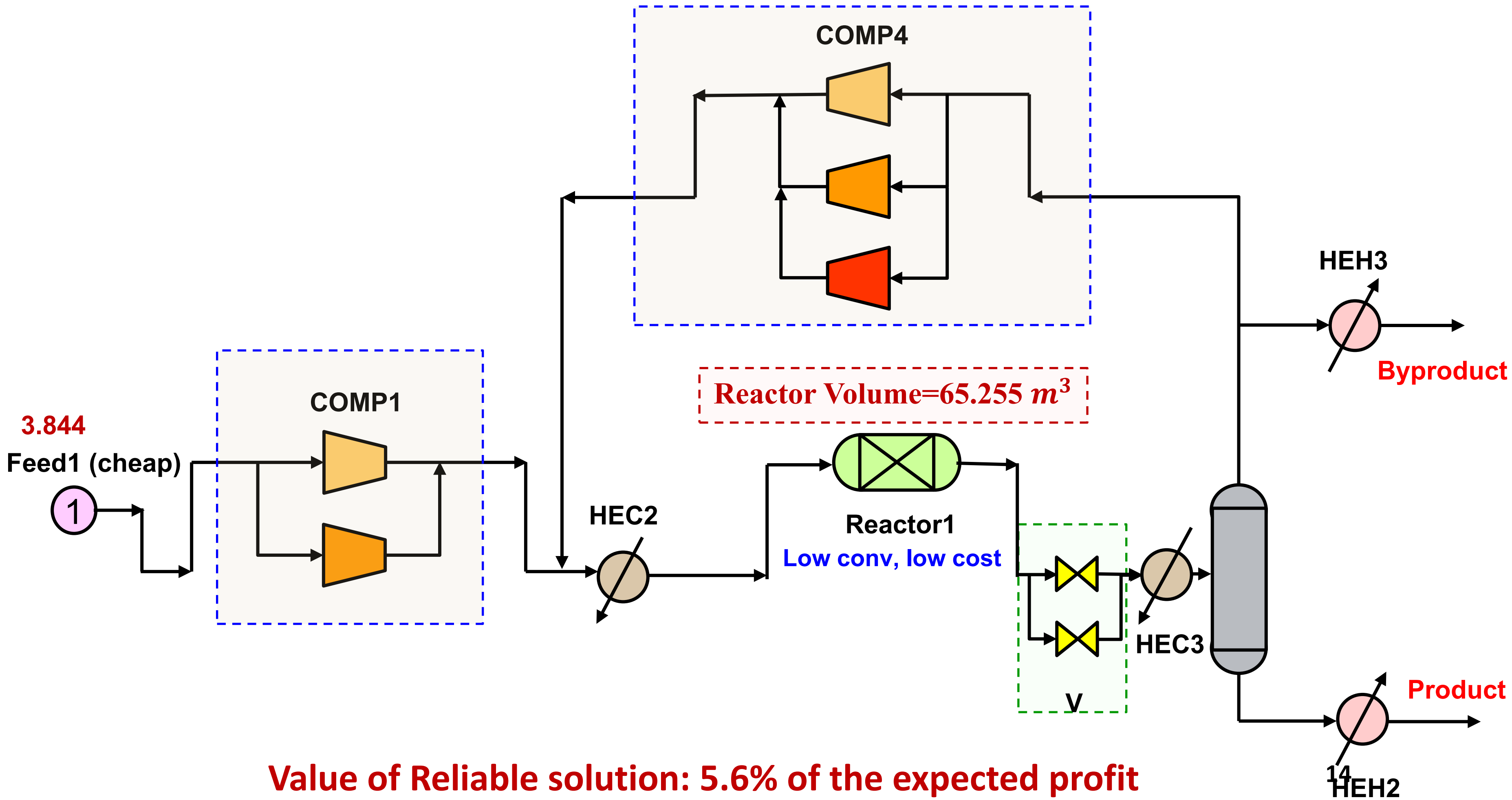


Industrial Methanol Synthesis

Stochastic Programming Model

Expected Profit = 3203.6879 ($1000 PER YEAR)

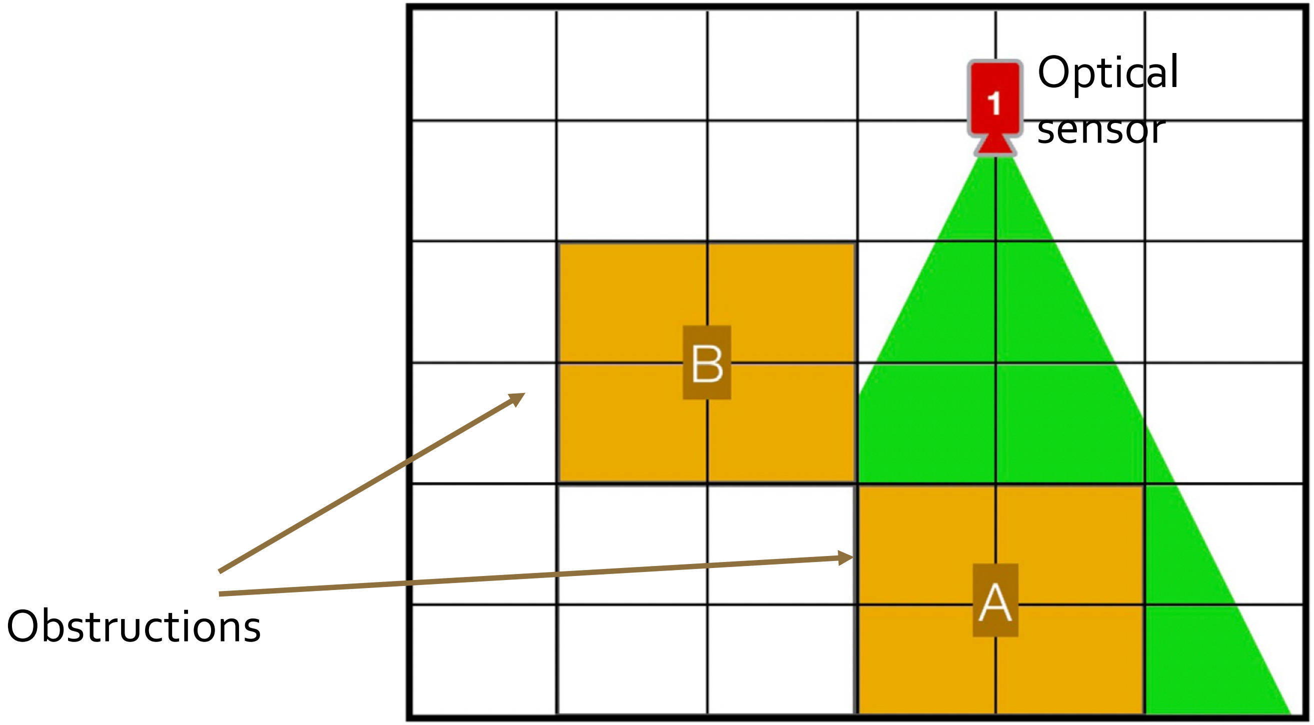
Consider demand uncertainty and reliability Simultaneously



Value of Reliable solution: 5.6% of the expected profit

Sensor Placement under Uncertainty

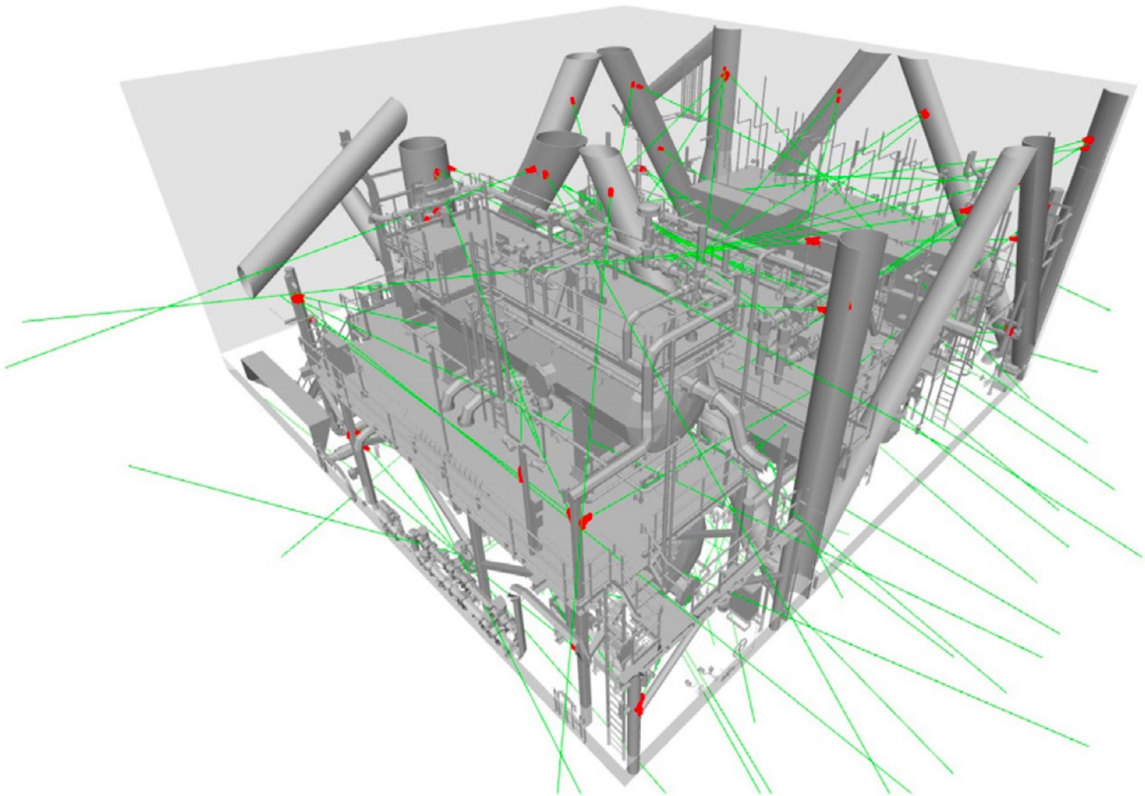
- Motivation: Determine the optimal configurations of sensors to maximize the probability of detecting safety hazards
- Flame, smoke, and heat detectors using chemical or optical sensors



Work of Prof. Carl Laird with P2SAC

Sensor Placement under Uncertainty

- Facility with 81 candidate flame detector locations (Kenexis Consulting Corporation)



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Mathematical Optimization for Sensor Placement

- Mixed-integer nonlinear programming (MINLP) formulation

Maximize expected coverage

$$\underset{x,\sigma}{\text{maximize}} \quad \sum_{e \in E} \sigma_e w_e$$

$$\text{subject to} \quad \sum_{l \in L} x_l \le k$$

Place at most k sensors

$$\sigma_e = 1 - 1[\prod_{l \in L_e} (1 - p_{l,e} x_l)] \qquad \forall e \in E$$

expected coverage of entity

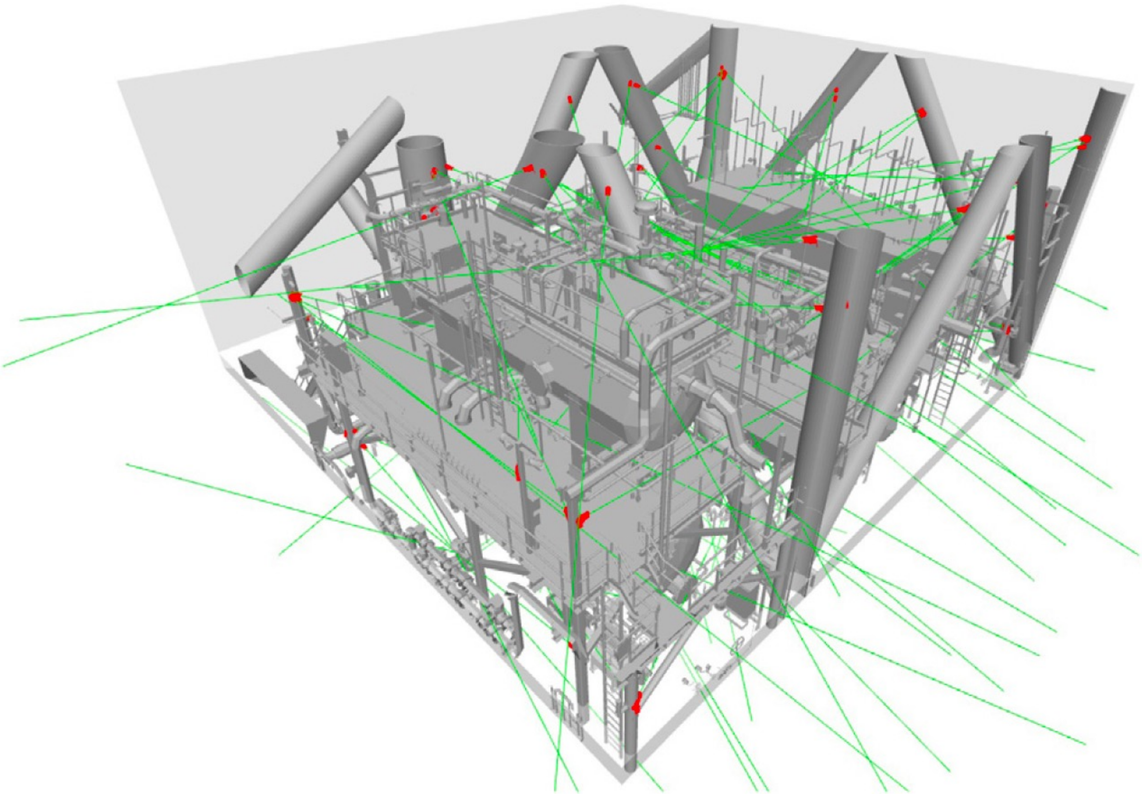
$$x_l \in \{0, 1\} \qquad \forall l \in L$$

$$0 \le \sigma_e \le 1 \qquad \forall e \in E$$

Binary variable, whether to place a sensor at location l

Sensor Placement under Uncertainty

- Facility with 81 candidate flame detector locations (Kenexis Consulting Corporation)
- Find the optimal configuration within 2 hours with a tailored algorithm



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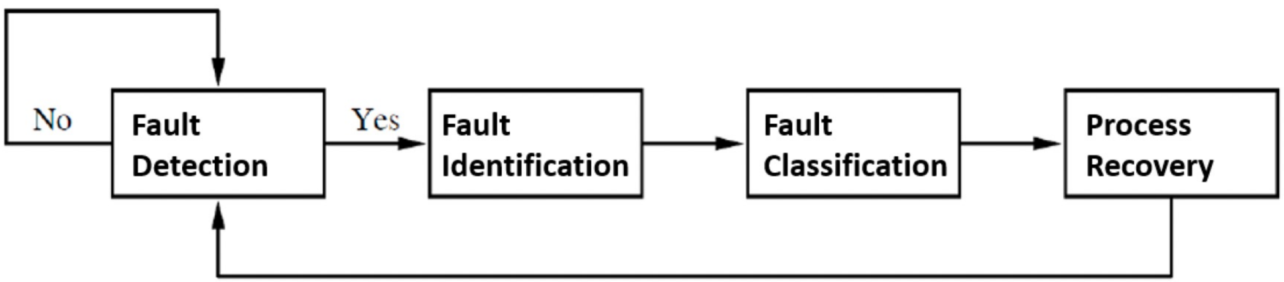
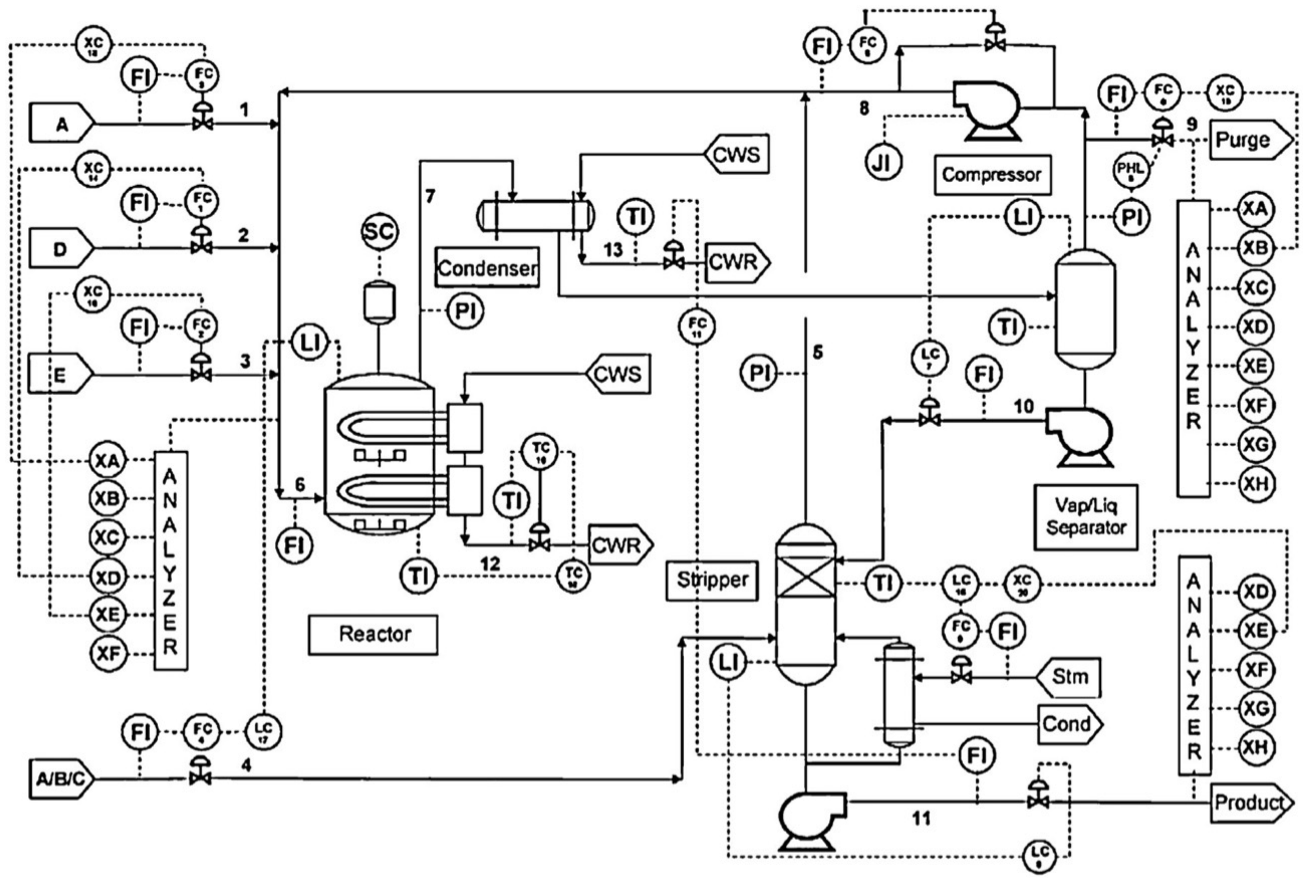
Machine Learning for Process Monitoring

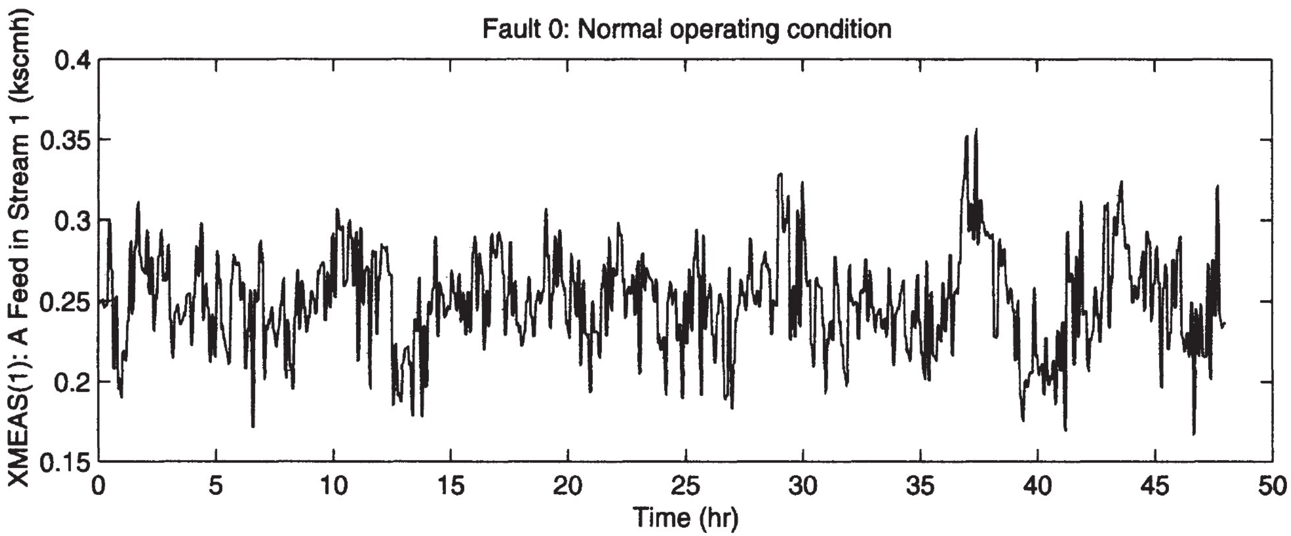


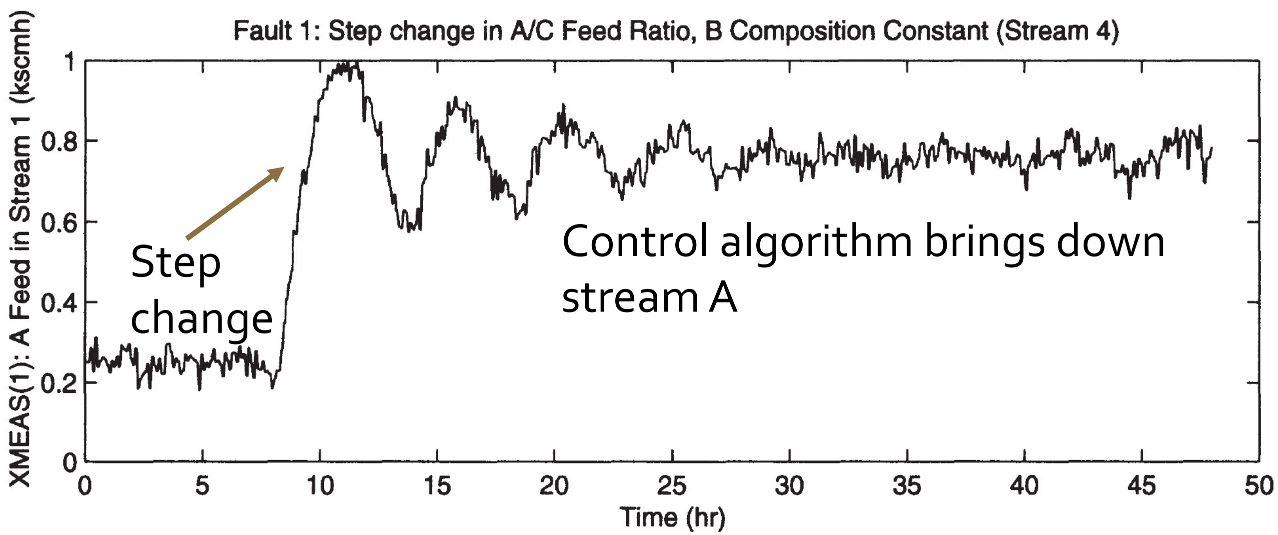
Tennessee Eastman process

- From measured state variables, perform fault detection



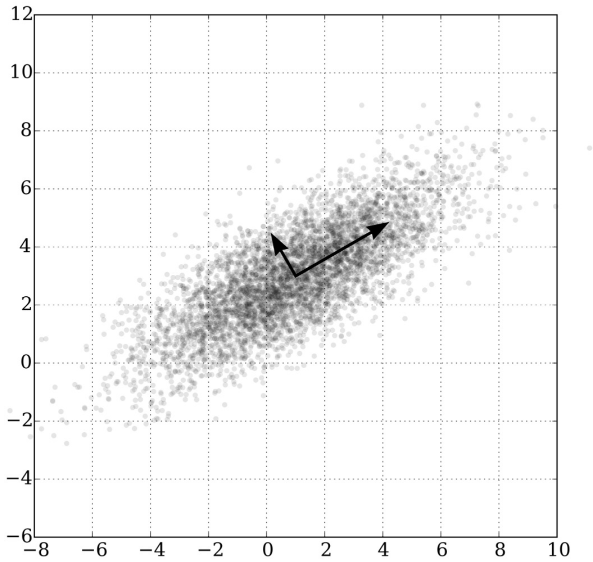
Example: Change in A/C Feed ratio

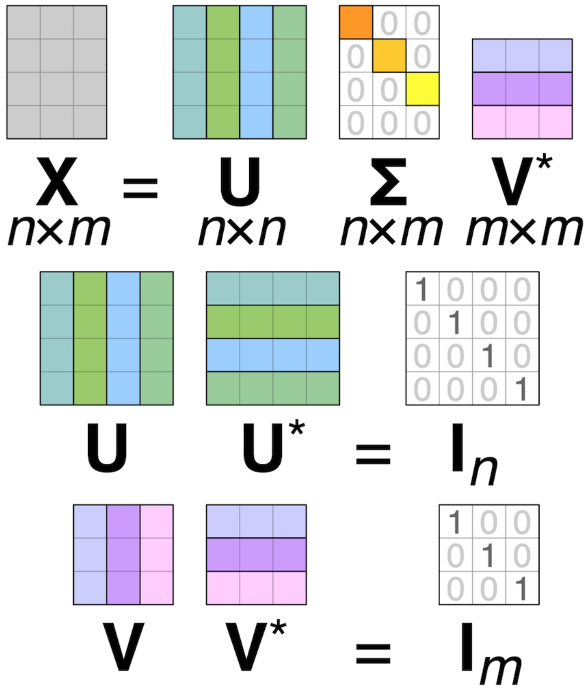




Classical Machine Learning Algorithm

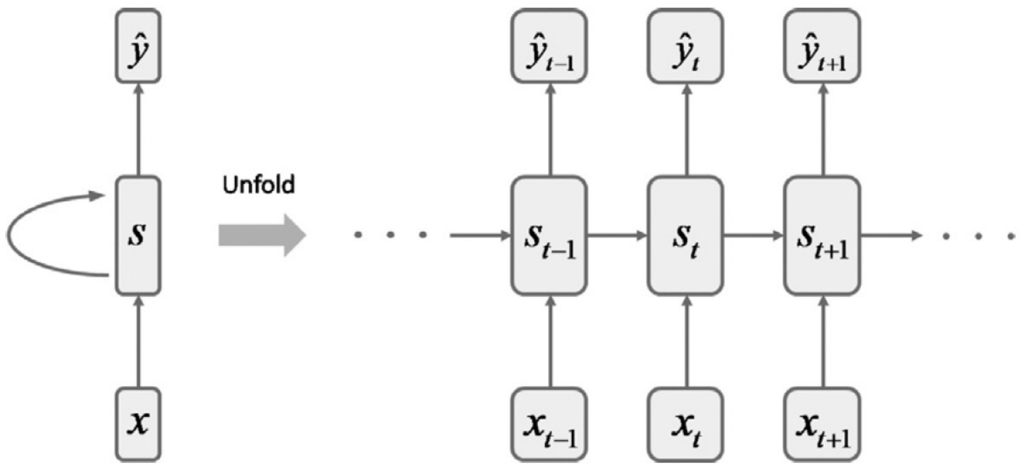
- Principal component analysis: identify the principal components where the data have the largest variance. The non-principal components are “noise”.
- Approach: singular value decomposition
- Pros: Interpretability
- Cons: Low accuracy for nonlinear processes.





Deep learning methods

- Recurrent neural network
- Pros: capable of handling nonlinearity and a high degree of spatio-temporal correlation
- Cons: hard to interpret



s_t:state

x_t: input

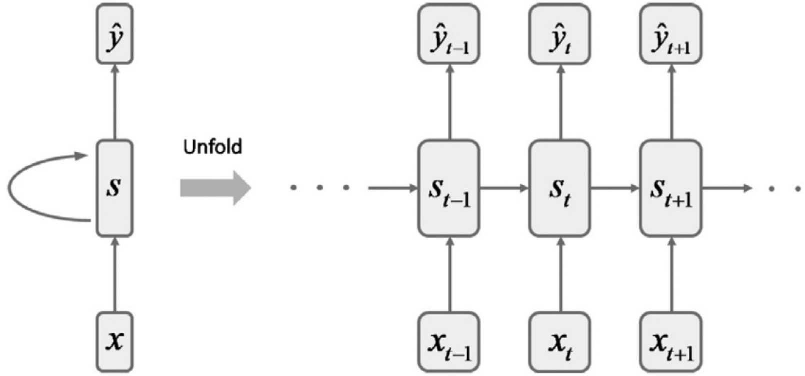
y_t: output

$$\boldsymbol{s}_t = f_s(\boldsymbol{x}_t, \boldsymbol{s}_{t-1} | \theta_s)$$
$$\hat{\boldsymbol{y}}_t = \boldsymbol{W}_y \boldsymbol{s}_t + \boldsymbol{b}_y$$

Explainable machine learning

- Ongoing research by PhD student Hao Chen

Machine learning-based models



Computationally efficient to use online
Hard to interpret

Physics-based models

$$\frac{dc}{dt} = \frac{F_0(c_0 - c)}{\pi r^2 h} - k_0 \exp\left(-\frac{E}{RT}\right) c$$

$$\frac{dT}{dt} = \frac{F_0(T_0 - T)}{\pi r^2 h} + \frac{-\Delta H}{\rho C_p} k_0 \exp\left(-\frac{E}{RT}\right) c + \frac{2U}{r \rho C_p}(T_c - T)$$

$$\frac{dh}{dt} = \frac{F_0 - F}{\pi r^2}$$

High fidelity but expensive to solve

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