Robust Optimization With Hybrid First-Principles Data-Driven Models

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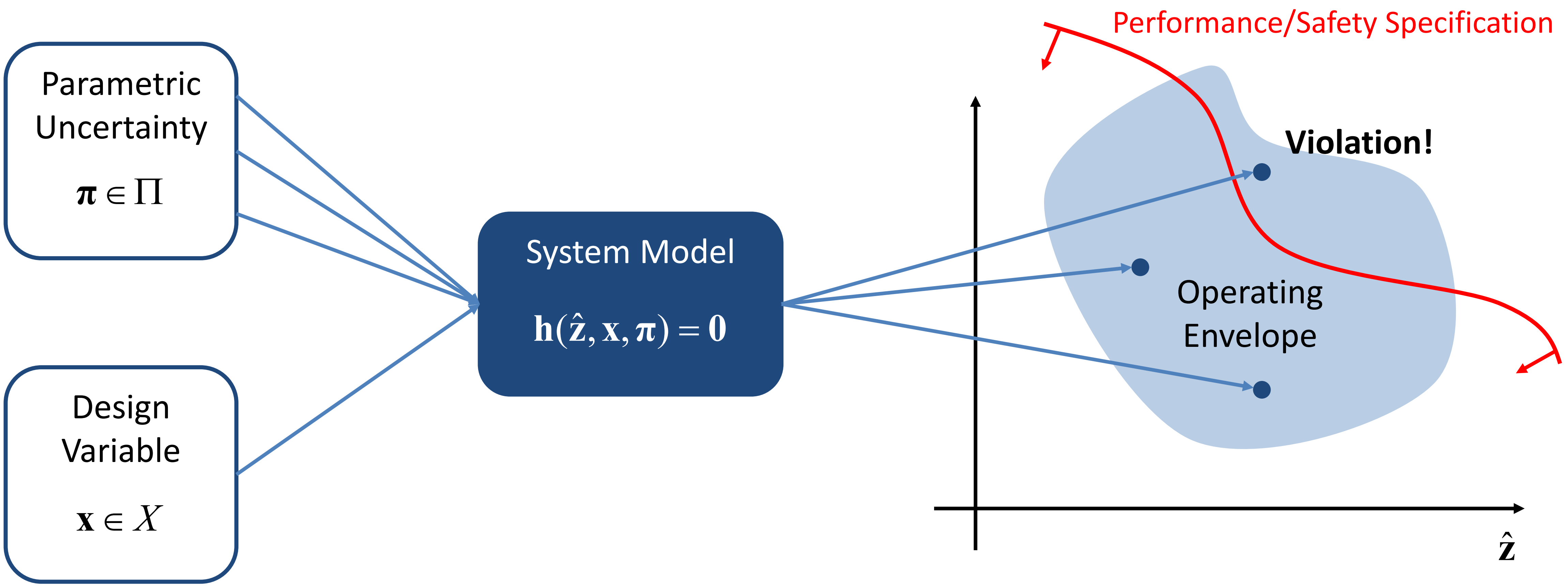
Process Systems and Operations Research Laboratory

Robust Optimization



Background

Process

Mechanism

Data

First-Principles Models
- Process mechanism is known
- Laws of nature are applied
- Idealized by assumptions

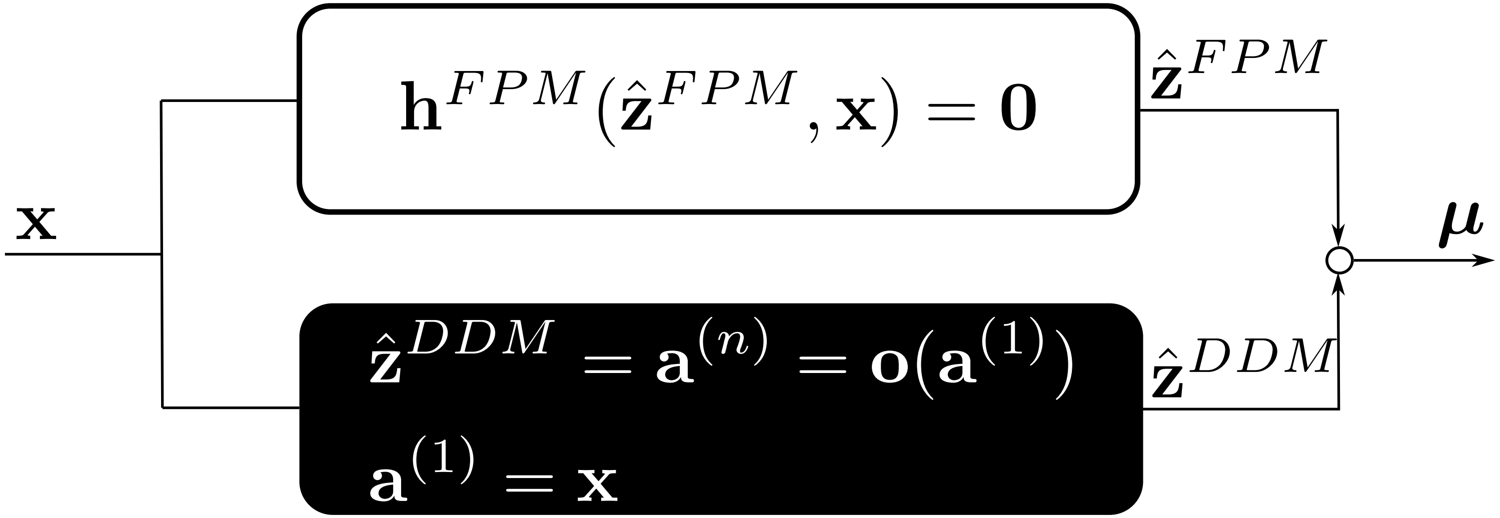
Hybrid Models
- Process knowledge is partially unknown
- Takes advantages of both

Data-Driven Models
- Input-output data inference
- No need for mechanism
- Valid within the domain

[1] von Stosch, M.; Oliveira, R.; Peres, J.; de Azevedo, S. F. Hybrid semi-parametric modeling in process systems engineering: Past, present and future. *Computers & Chemical Engineering* 2014,60, 86–101.

Hybrid Model Architecture

- Parallel structure



Hybrid Model Architecture

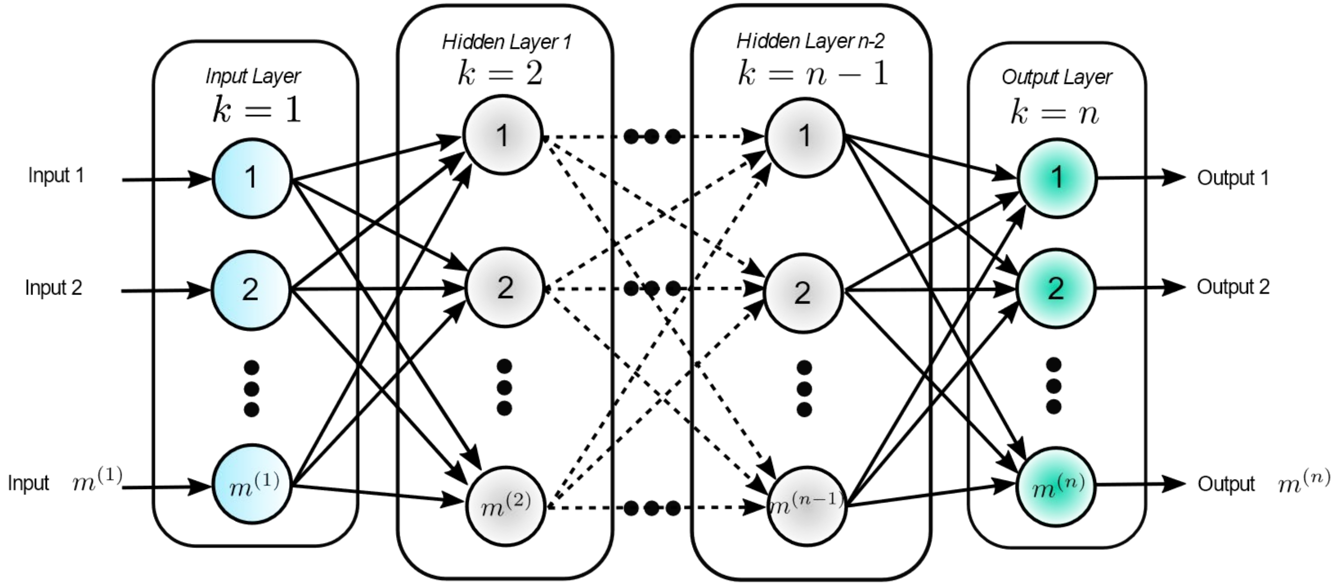
- Serial structure

$$\mathbf{x} \longrightarrow \boxed{\begin{aligned} \hat{\mathbf{z}}^{DDM} &= \mathbf{a}^{(n)} = \mathbf{o}(\mathbf{a}^{(1)}) \\ \mathbf{a}^{(1)} &= \mathbf{x} \end{aligned}} \xrightarrow{\hat{\mathbf{z}}^{DDM}} \boxed{\mathbf{h}^{FPM}(\hat{\mathbf{z}}^{FPM}, \hat{\mathbf{z}}^{DDM}) = \mathbf{0}} \xrightarrow{\hat{\mathbf{z}}^{FPM}}$$

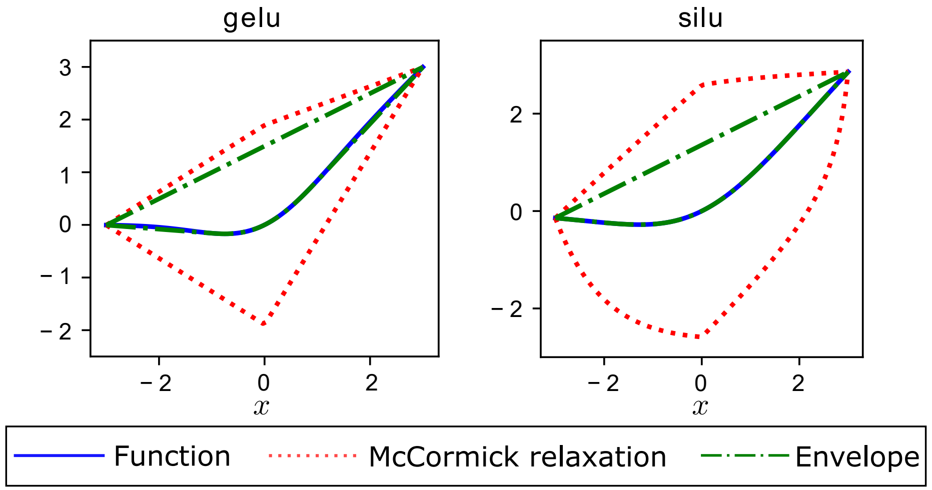
$$\mathbf{x} \longrightarrow \boxed{\mathbf{h}^{FPM}(\hat{\mathbf{z}}^{FPM}, \mathbf{x}) = \mathbf{0}} \xrightarrow{\hat{\mathbf{z}}^{FPM}} \boxed{\begin{aligned} \hat{\mathbf{z}}^{DDM} &= \mathbf{a}^{(n)} = \mathbf{o}(\mathbf{a}^{(1)}) \\ \mathbf{a}^{(1)} &= \hat{\mathbf{z}}^{FPM} \end{aligned}} \xrightarrow{\hat{\mathbf{z}}^{DDM}}$$

Artificial Neural Network

- Multilayer perceptron



- Convex/concave envelopes of activation functions



Equality-Constrained Bilevel program

Bilevel Program

$$
\begin{aligned}
f^* = \;& \min_{\mathbf{x}\in X} f(\mathbf{x}) \\
\text{s.t.} \;& 0 \geq \max_{\boldsymbol{\pi}\in\Pi,\hat{\mathbf{z}}\in Z} g(\hat{\mathbf{z}},\mathbf{x},\boldsymbol{\pi}) \\
& \qquad \text{s.t. } \mathbf{h}(\hat{\mathbf{z}},\mathbf{x},\boldsymbol{\pi}) = \mathbf{0}
\end{aligned}
$$

Design under uncertainty feasibility problem

$$
\begin{aligned}
\gamma^* = \;& \min_{\mathbf{x}\in X,\gamma\in\mathbb{R}} \gamma \\
\text{s.t.} \;& \gamma = \max_{\boldsymbol{\pi}\in\Pi,\hat{\mathbf{z}}\in Z} g(\hat{\mathbf{z}},\mathbf{x},\boldsymbol{\pi}) \\
& \qquad \text{s.t. } \mathbf{h}(\hat{\mathbf{z}},\mathbf{x},\boldsymbol{\pi}) = \mathbf{0}
\end{aligned}
$$

Optimal design under uncertainty problem

$$
\begin{aligned}
f^* = \;& \min_{\mathbf{x}\in X} f(\mathbf{x}) \\
\text{s.t.} \;& 0 \geq \max_{\boldsymbol{\pi}\in\Pi,\hat{\mathbf{z}}\in Z} g(\hat{\mathbf{z}},\mathbf{x},\boldsymbol{\pi}) \\
& \qquad \text{s.t. } \mathbf{h}(\hat{\mathbf{z}},\mathbf{x},\boldsymbol{\pi}) = \mathbf{0}
\end{aligned}
$$

Operation under uncertainty feasibility problem

$$
\begin{aligned}
\gamma^* = \;& \max_{\boldsymbol{\pi}\in\Pi,\gamma\in\mathbb{R}} \gamma \\
\text{s.t.} \;& \gamma = \min_{\mathbf{x}\in X,\hat{\mathbf{z}}\in Z} g(\hat{\mathbf{z}},\mathbf{x},\boldsymbol{\pi}) \\
& \qquad \text{s.t. } \mathbf{h}(\hat{\mathbf{z}},\mathbf{x},\boldsymbol{\pi}) = \mathbf{0}
\end{aligned}
$$

Reformulation: Semi-Infinite Program

- How to solve the min-max problems?
  - Assume there exists a unique implicit function $\mathbf{z}: X \times \Pi \rightarrow Z$ such that

$$\mathbf{h}(\mathbf{z}(\mathbf{x}, \boldsymbol{\pi}), \mathbf{x}, \boldsymbol{\pi}) = \mathbf{0}$$

  - Use equivalent semi-infinite constraints for the lower-level program:

$$0 \geq \max_{\boldsymbol{\pi} \in \Pi, \hat{\mathbf{z}} \in Z} g(\hat{\mathbf{z}}, \mathbf{x}, \boldsymbol{\pi}) \Leftrightarrow g(\mathbf{z}(\mathbf{x}, \boldsymbol{\pi}), \mathbf{x}, \boldsymbol{\pi}) \leq 0, \forall \boldsymbol{\pi} \in \Pi$$

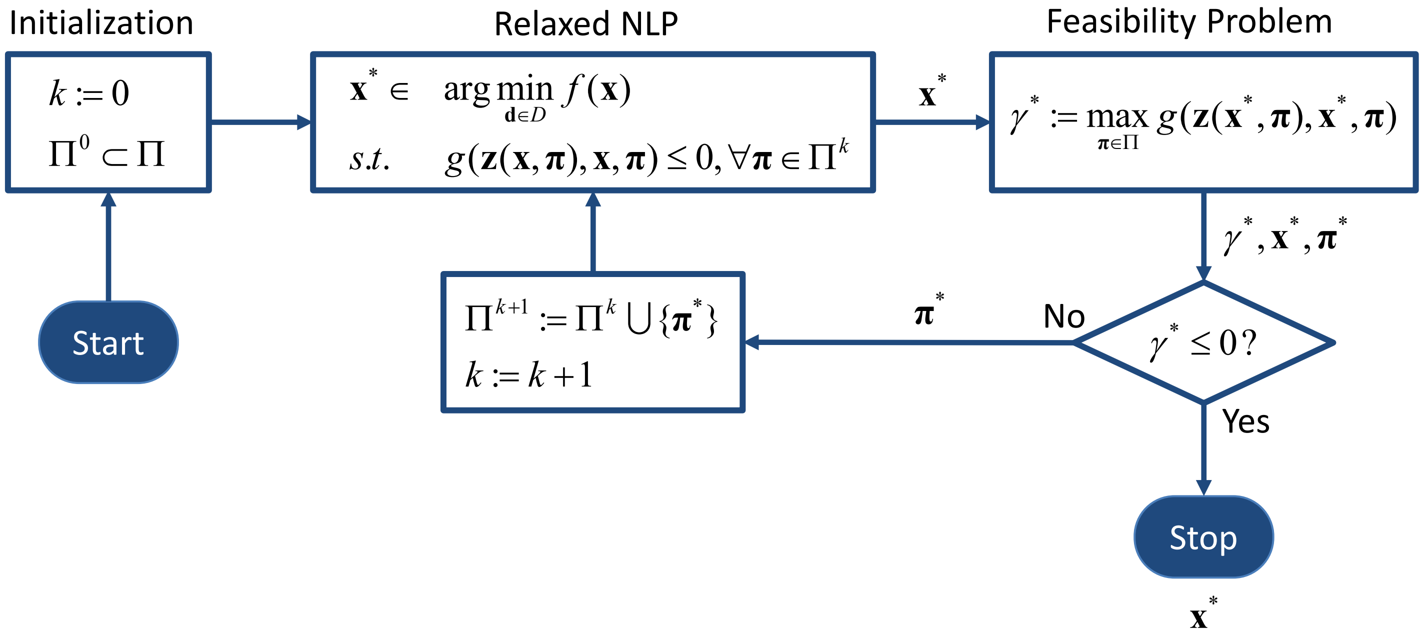
  - Then, the min-max program can be reformulated as a semi-infinite program (SIP):

$$\begin{aligned} &\min_{\mathbf{x} \in X} f(\mathbf{x}) \\ \text{s.t.} \quad &0 \geq \max_{\boldsymbol{\pi} \in \Pi, \hat{\mathbf{z}} \in Z} g(\hat{\mathbf{z}}, \mathbf{x}, \boldsymbol{\pi}) \\ &\qquad \text{s.t.} \;\; \mathbf{h}(\hat{\mathbf{z}}, \mathbf{x}, \boldsymbol{\pi}) = \mathbf{0} \end{aligned} \quad \Leftrightarrow \quad \begin{aligned} &\min_{\mathbf{x} \in X} f(\mathbf{x}) \\ \text{s.t.} \quad &g(\mathbf{z}(\mathbf{x}, \boldsymbol{\pi}), \mathbf{x}, \boldsymbol{\pi}) \leq 0, \boxed{\forall \boldsymbol{\pi} \in \Pi} \end{aligned}$$

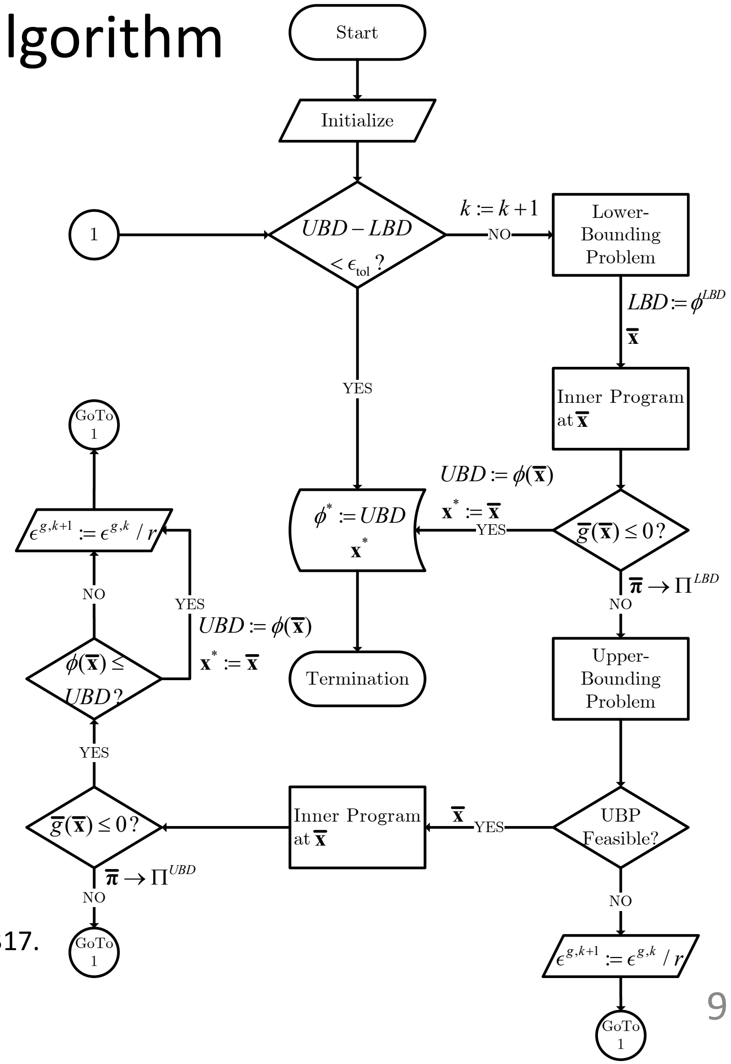
Π is a nonempty, compact interval,
there are infinitely-many constraints

SIP Algorithm

- Cutting plane algorithm

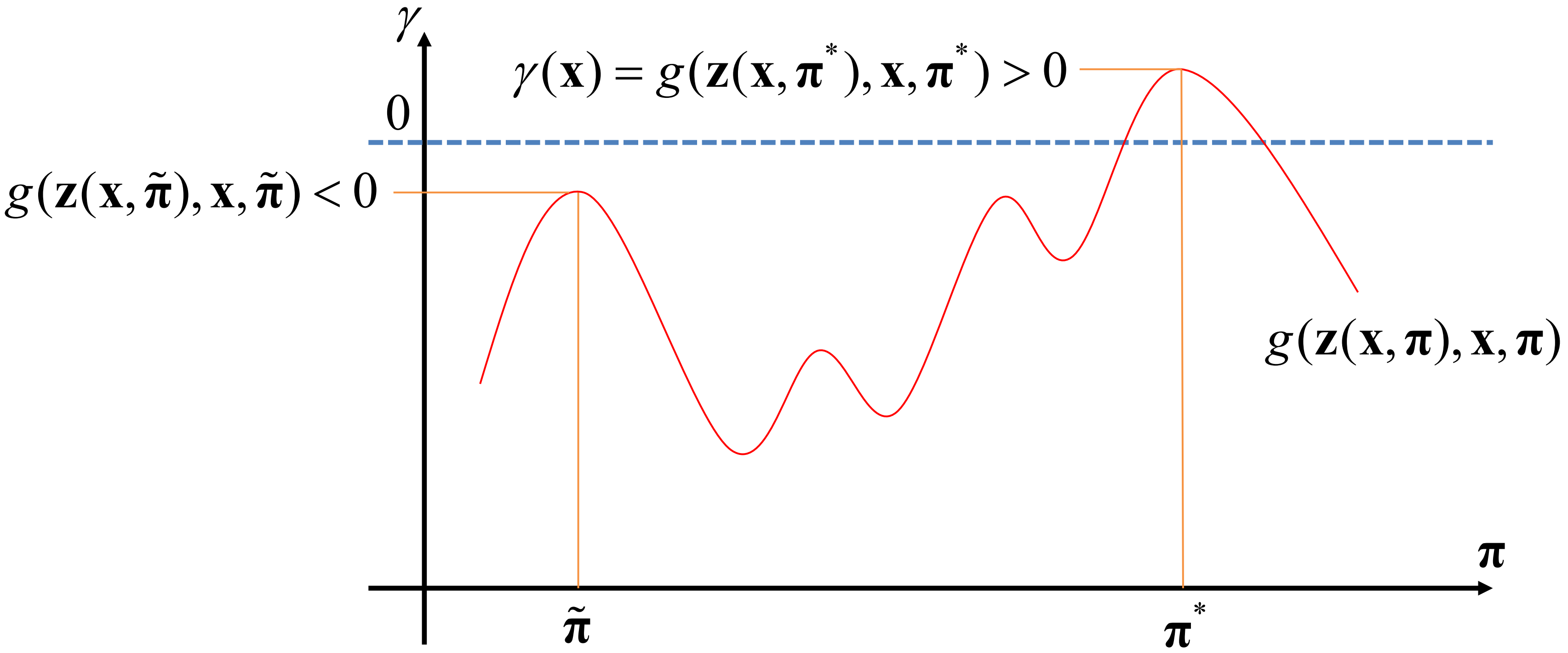


- SIPres algorithm



[1] Blankenship, J. W.; Falk, J. E. Infinitely constrained optimization problems. J. *Optim*. Theory Appl. 1976, 19.
[2] Mitsos, A. Global optimization of semi-infinite programs via restriction of the right-hand side. *Optimization* 2011, 60, 1291–1308.
[3] Stuber, M. D.; Barton, P. I. Semi-Infinite Optimization with Implicit Functions. *Industrial& Engineering Chemistry Research* 2014,54, 307–317.

Global Optimization



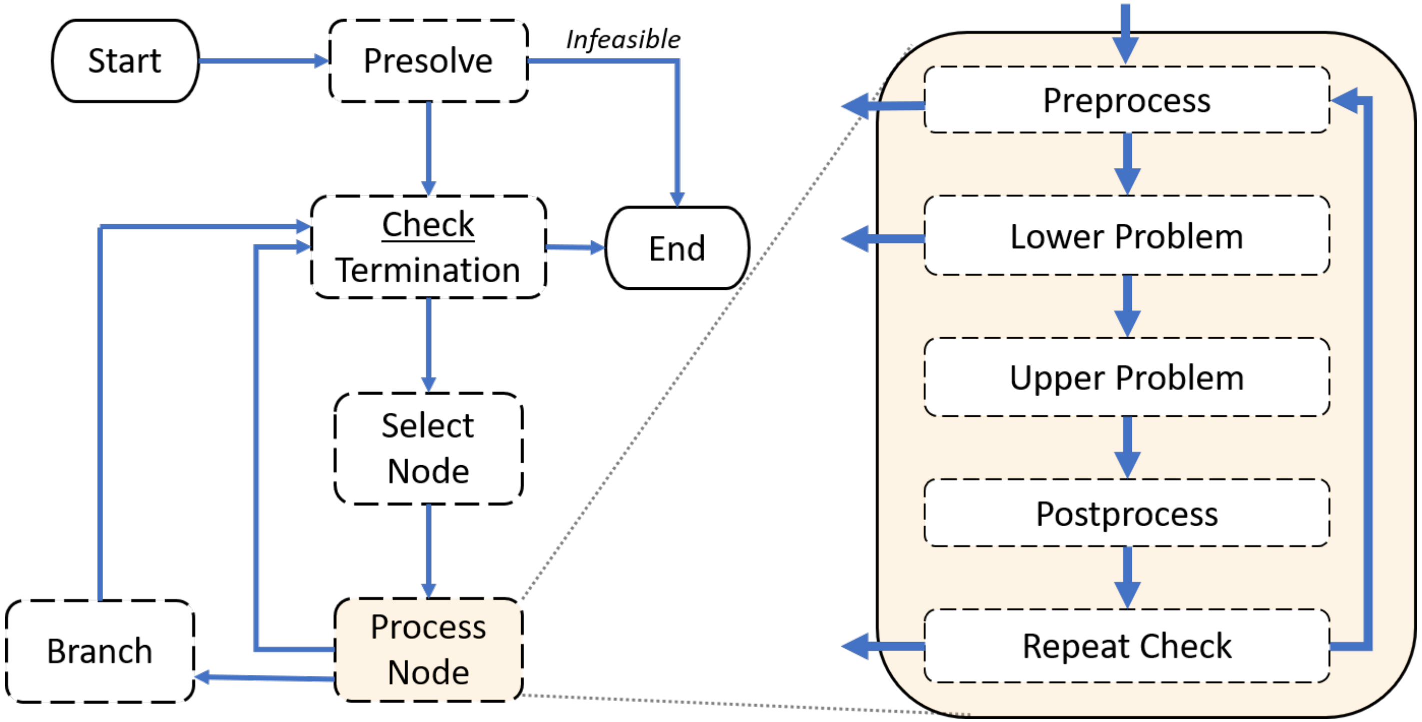
A global solution is required

$$\gamma(\mathbf{x}) = \max_{\boldsymbol{\pi}\in\Pi} g(\mathbf{z}(\mathbf{x},\boldsymbol{\pi}),\mathbf{x},\boldsymbol{\pi})$$

- Every realization of uncertainty should be considered
- Functions are likely nonconvex, global solution is required

EAGO.jl: Global Deterministic Optimization of Simulations

- EAGO.jl: A deterministic global optimizer in Julia

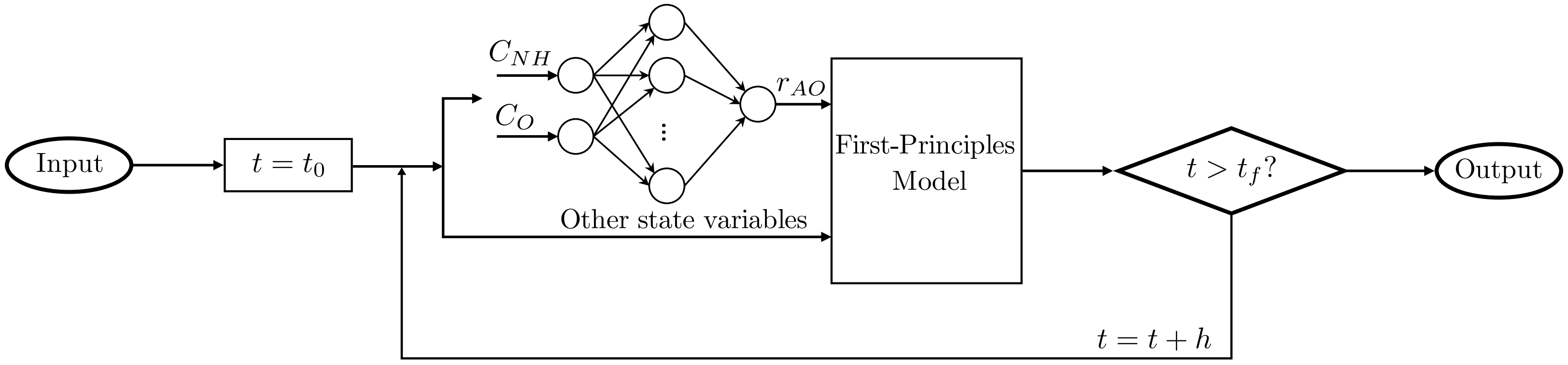


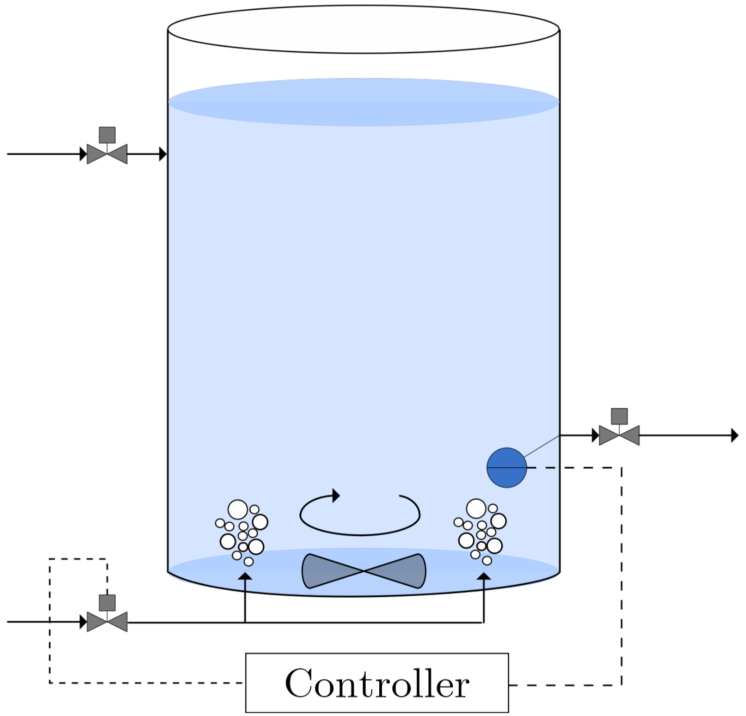
https://www.github.com/PSORLab/EAGO.jl

- Can solve formulations with user-defined expressions (simulations, etc.)
- Uses composite relaxation framework that enables expansion to an esoteric set of problems
- Includes a full library of envelopes for activation functions and other common expressions/transcendental functions

1. Wilhelm, M.E., and Stuber, M.D.. **EAGO.jl: easy advanced global optimization in Julia.** *Optimization Methods and Software*, 1-26.

Case Study: Nitrification CSTR





Model:

$$\frac{dC_{NH}}{dt} = \frac{1}{V}(\dot{m}_{in}C_{in} - \dot{m}_{out}C_{NH}) - r_{AO} \cdot X_{AO}$$

$$\frac{dC_{NI}}{dt} = r_{AO} \cdot X_{AO} - r_{NO} \cdot X_{NO}$$

$$\frac{dC_{NA}}{dt} = r_{NO} \cdot X_{NO}$$

$$\frac{dC_O}{dt} = -r_{AO} \cdot \Psi_{AO} \cdot X_{AO} - r_{NO} \cdot \Psi_{NO} \cdot X_{NO} + \boxed{k_{la}} \cdot (C_O^* - C_O)$$

$$\boxed{\frac{0.2967Q \cdot \mathrm{SOTE}}{C_O^* \cdot V}}$$

Robust design:

$$\phi^* = \min_{d \in D} d$$

$$\text{s.t.} \quad \max\{C_{NH}(t_f, d, p) - \mathrm{USL_{NH}}, C_O(t_f, d, p) - \mathrm{USL_O}\}, \forall p \in P$$

Solution	Time
$d^* = 535$	83 s

Case Study: Subsea Separators

Inlet Specification

$$SG_O = \frac{141.5}{131.5 + API}$$

$$SG_{mix} = (\xi_{G1}/SG_G + \xi_{W1}/SG_W + \xi_{O1}/SG_O)^{-1}$$

$$\xi_{G1} + \xi_{W1} + \xi_{O1} = 1$$

Valve 2

$$P_5 = P_{LLS}$$

$$\xi_4 = \xi_5$$

$$\dot{m}_4 = \dot{m}_5 = u_2 C_{v2} \sqrt{\frac{P_4 - P_5}{\rho_4 / \rho_W{}^o}}$$

Gas Mixer

$$\xi_4 = \xi_5$$

$$\dot{m}_9 = \dot{m}_3 + \dot{m}_8$$

$$P_9 = \min(P_3, P_8)$$

Gas-Liquid Separator

$$\xi_3 = (1,0,0), \quad \xi_{G4} + \xi_{O4} + \xi_{W4} = 1$$

$$\dot{m}_2 = \dot{m}_3 + \dot{m}_4, \quad \xi_{G2}\dot{m}_2 = \xi_{G3}\dot{m}_3 + \xi_{G4}\dot{m}_4, \quad \xi_{W2}\dot{m}_2 = \xi_{W4}\dot{m}_4$$

$$\xi_{G4} = \xi_{G2} \exp\left[-k_{GLS} \frac{V_{GLS}}{\dot{m}_4 / \rho_4}\right]$$

$$\rho_4 = \rho_W{}^o (\xi_{G4}/SG_G + \xi_{W4}/SG_W + \xi_{O4}/SG_O)^{-1}, \quad P_3 = P_2, \quad P_4 = P_3 + \rho_4 g_a H_{GLS}$$

$$V_{GLS} = L_{GLS}\left((H_{GLS} - R_{GLS})\sqrt{2R_{GLS}H_{GLS} - H_{GLS}{}^2} + R_{GLS}{}^2 \boxed{\cos^{-1}\left[1 - \frac{H_{GLS}}{R_{GLS}}\right]}\right)$$

$$\dot{m}_2 \ \& \ \xi_2 \quad wellhead - specification$$

Domain violation

Liquid-Liquid Separator

$$\xi_6 = (0,1,0), \quad \xi_8 = (1,0,0), \quad \xi_{G7} + \xi_{O7} = 1$$

$$\dot{m}_5 = \dot{m}_6 + \dot{m}_7 + \dot{m}_8, \quad \xi_{G5}\dot{m}_5 = \xi_{G8}\dot{m}_8 + \xi_{G7}\dot{m}_7, \quad \xi_{W5}\dot{m}_5 = \xi_{W6}\dot{m}_6$$

$$\xi_{G7} = \xi_{G5} \exp\left[-k_{LLS} \frac{V_{oil}}{\dot{m}_7 / \rho_7}\right]$$

$$\rho_7 = \rho_W{}^o (\xi_{G7}/SG_G + \xi_{O7}/SG_O)^{-1}, \quad P_8 = P_{LLS}$$

$$V_{oil} = V_{LLS}\left(\frac{\dot{m}_7}{\rho_7}\frac{\rho_5}{\dot{m}_5}\right)$$

$$V_{LLS} = L_{LLS}\left((H_{LLS} - R_{LLS})\sqrt{2R_{LLS}H_{LLS} - H_{LLS}{}^2} + R_{LLS}{}^2 \cos^{-1}\left[1 - \frac{H_{LLS}}{R_{LLS}}\right]\right)$$

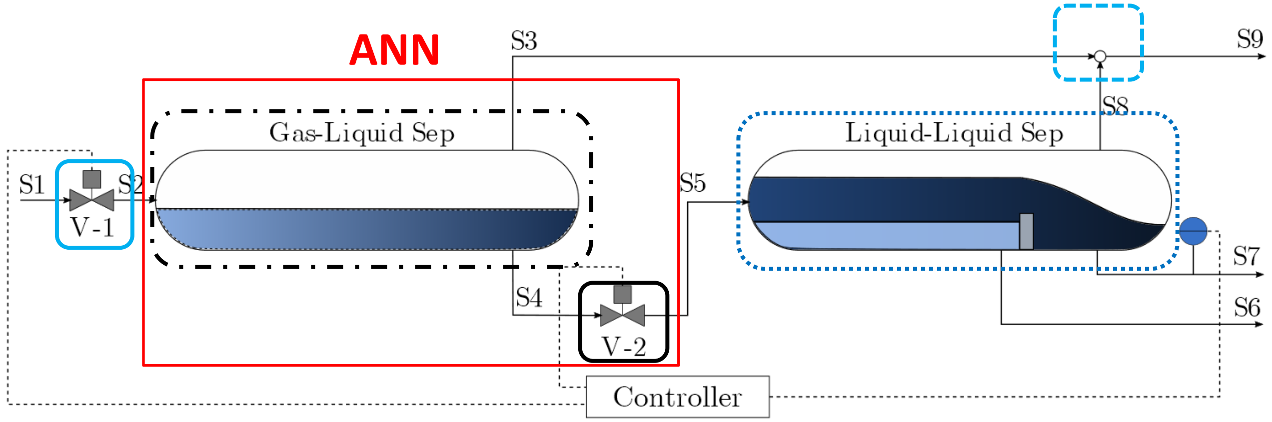
Valve 1

$$P_1 = P_{well}$$

$$P_2 = P_{GLS}$$

$$\xi_1 = \xi_2$$

$$\dot{m}_1 = \dot{m}_2 = u_1 C_{v1}\sqrt{\frac{P_1 - P_2}{SG_{mix}}}$$



[1] **Worst-case design of subsea production facilities using semi-infinite programming.** Stuber, M.D. et al. (2014) *AIChE Journal*, 60, 2513-2524

Case Study: Subsea Separators

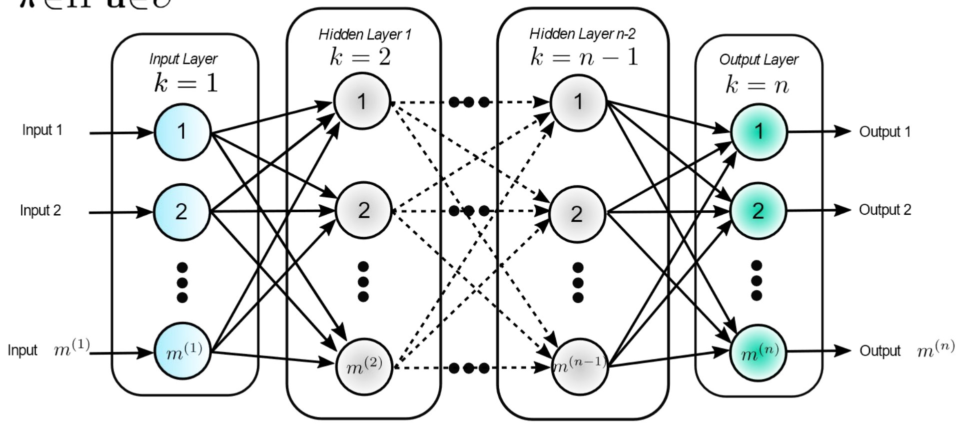
Problem Statement

For any inlet gas fraction (*stream 1*) within typical bounds, is there a control setting that will prevent the effluent gas fraction of the liquid-liquid separator (*stream 7*) from exceeding the specification and damaging the pump.

Problem Statement (Max-Min-Max Program)

$$\mathbf{h}(\mathbf{z},\mathbf{u},\boldsymbol{\pi}) = \mathbf{0} \longrightarrow \mathbf{z} = \mathrm{x}(\mathbf{u},\boldsymbol{\pi})$$

$$\max_{\boldsymbol{\pi}\in\Pi} \min_{\mathbf{u}\in U} \max \{g(\mathbf{z}(\mathbf{u},\boldsymbol{\pi}),\mathbf{u},\boldsymbol{\pi}), g_c(\mathbf{z}(\mathbf{u},\boldsymbol{\pi}),\mathbf{u},\boldsymbol{\pi})\} \leq 0.$$



Semi-infinite constraint:

$$g(\mathbf{x}(\mathbf{u},\boldsymbol{\pi}),\mathbf{u},\boldsymbol{\pi}) \equiv x_{G7}(\mathbf{u},\boldsymbol{\pi}) - 0.05 \leq 0$$

Uncertain Parameter (Inlet Gas Fraction)

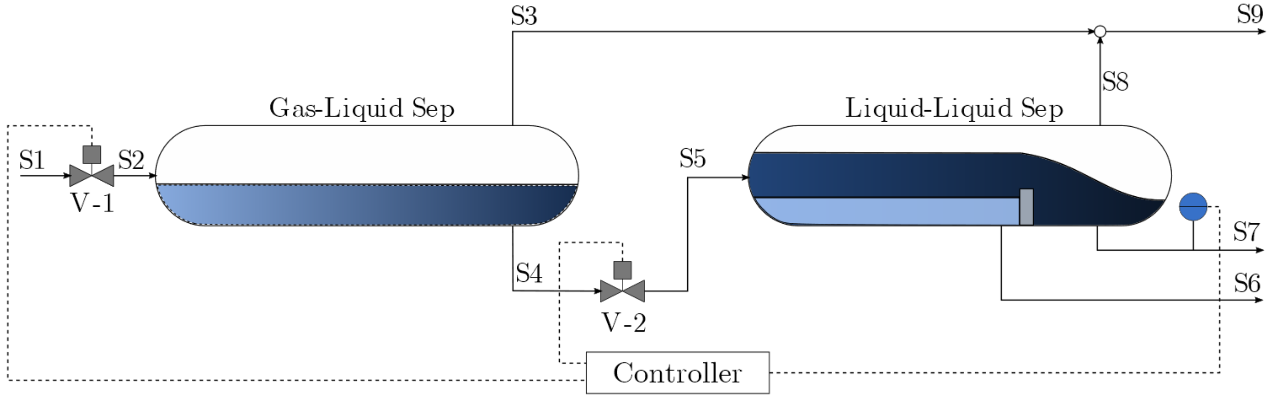
$$\boldsymbol{\pi} = (\xi_{G1}) \in [0.35, 0.5]$$

Control Settings (Valve Position)

$$\mathbf{u} = (u_1, u_2) \in [0.3, 0.85] \times [0.3, 0.85]$$

State Variables

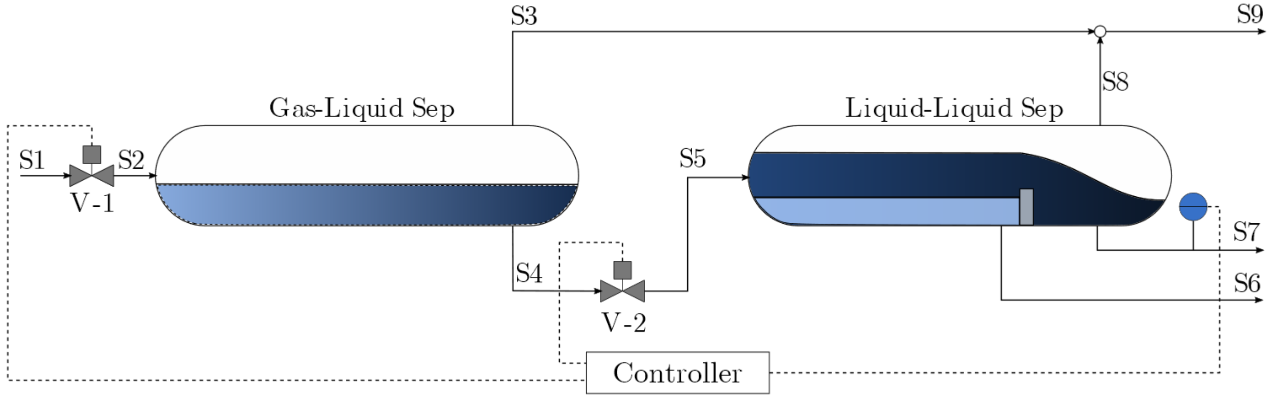
$$\mathbf{z} = \left(\xi_{G4}, \xi_{W4}, \xi_{O4}, \xi_{G7}, \xi_{O7}, H_{GLS}, \dot{m}_3, \dot{m}_4, \dot{m}_6, \dot{m}_7, \dot{m}_8\right)$$



[1] Worst-case design of subsea production facilities using semi-infinite programming. Stuber, M.D. et al. (2014) *AIChE Journal*, 60, 2513-2524

Case Study: Subsea Separators

- The part of the simulation not replaced with surrogate models was evaluated in a block sequential fashion.
- Solved using the SIPres[1] in EAGO[2] to an absolute tolerance of 10^{-3}.
- Optimal solution found at -6.6×10^{-4}, ensure the robust feasibility.
- The algorithm terminated within an optimal value in 3 iterations, taking 2.9 CPU seconds.
- Results in a 70x improvement in computational time relative to implicit function method used with original simulation in [1].



[1] Worst-case design of subsea production facilities using semi-infinite programming. Stuber, M.D. et al. (2014) *AIChE Journal*, 60, 2513-2524

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Any questions?

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