



• AUGUST 2026

SAFE EXPLORATION IN NONLINEAR PROCESSES

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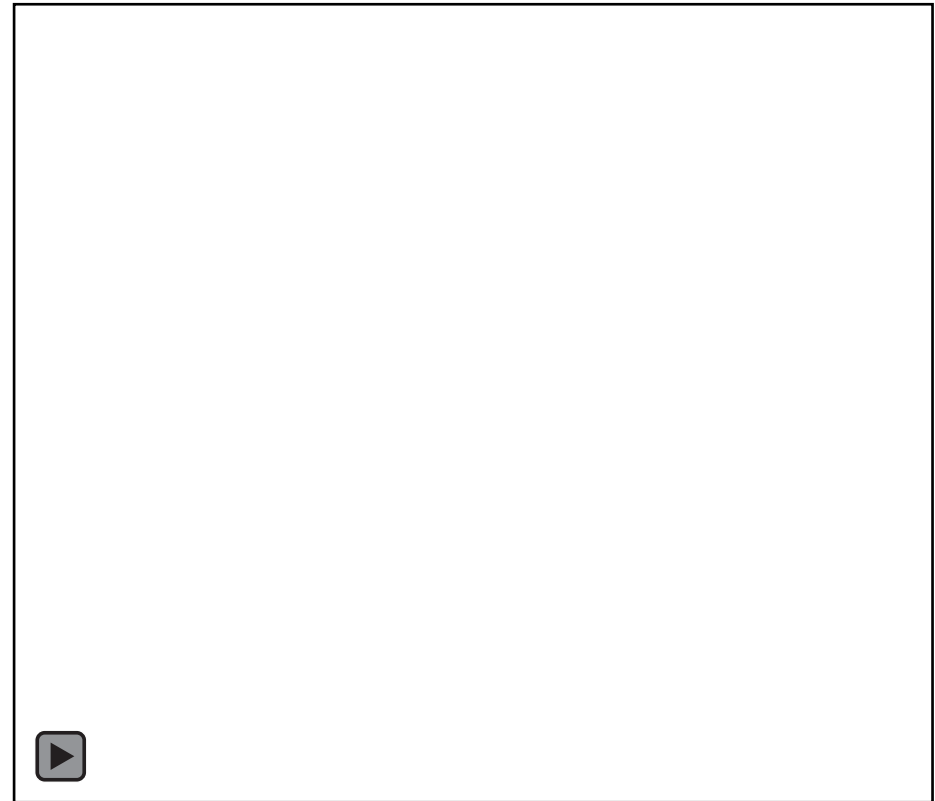
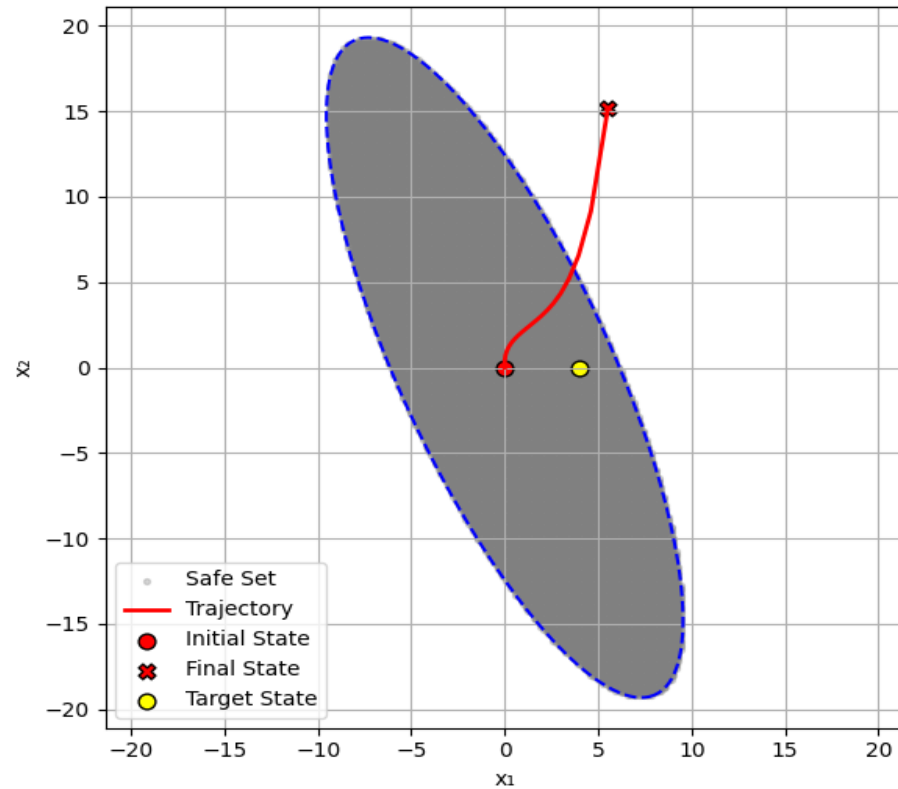
ENGINEERED
TO OUTRUN

Agenda

- Problem Formulation:
 - What do we mean by safe exploration?
 - How to use the explored data?
- Methodology
 - Toy example of a simple system
 - Benchmark control example (3×3)
- Industrial application
 - Two-phase separator
- Conclusion
 - Advantages
 - Limitations

Problem Formulation

What do we mean by safe exploration?



Problem Formulation

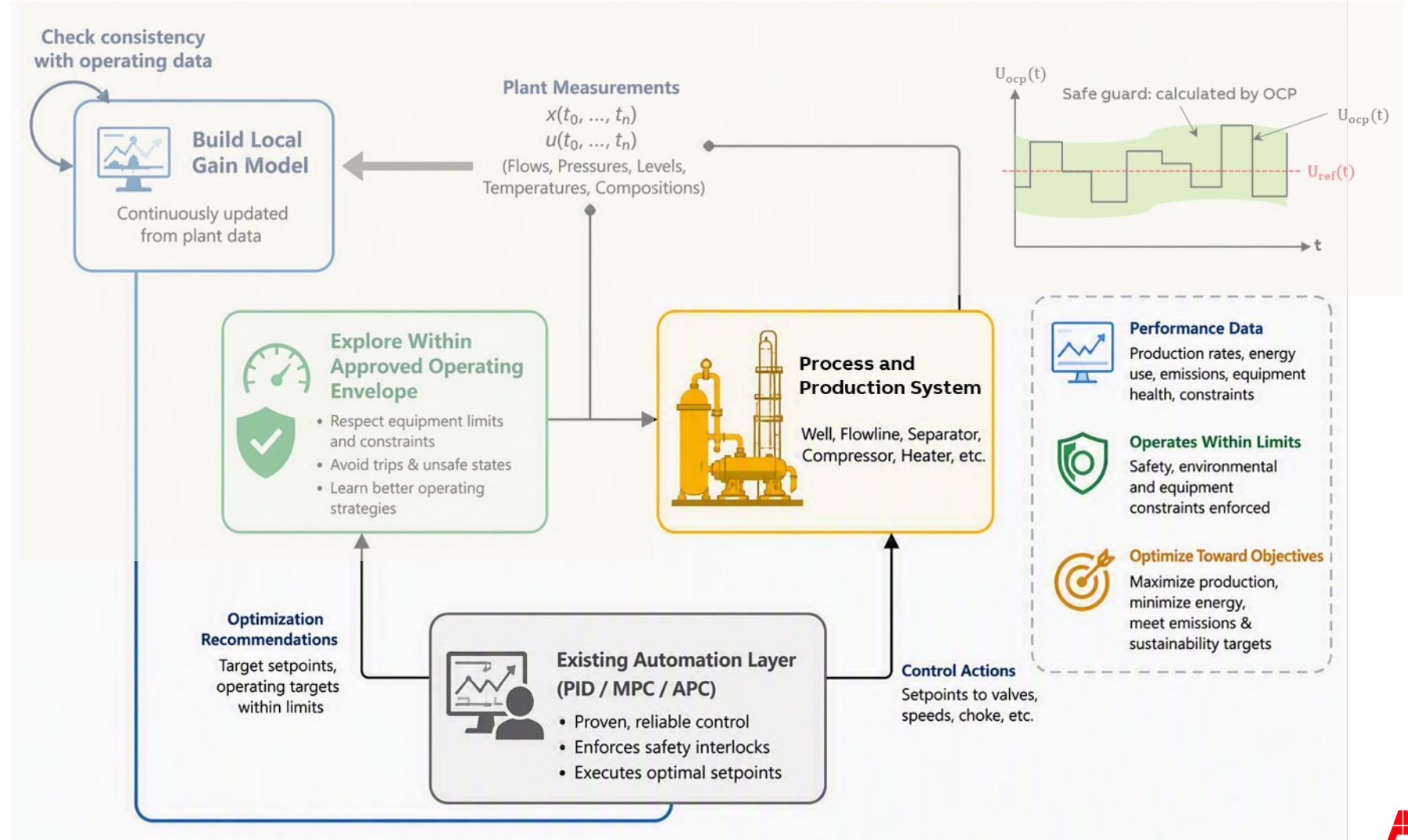
How to use the explored data?

1. Build process models
2. Optimize operations
3. Controller Tuning
4. Train ML/AI models
5. Alarm rationalization?

Problem Formulation

How to use the explored data?

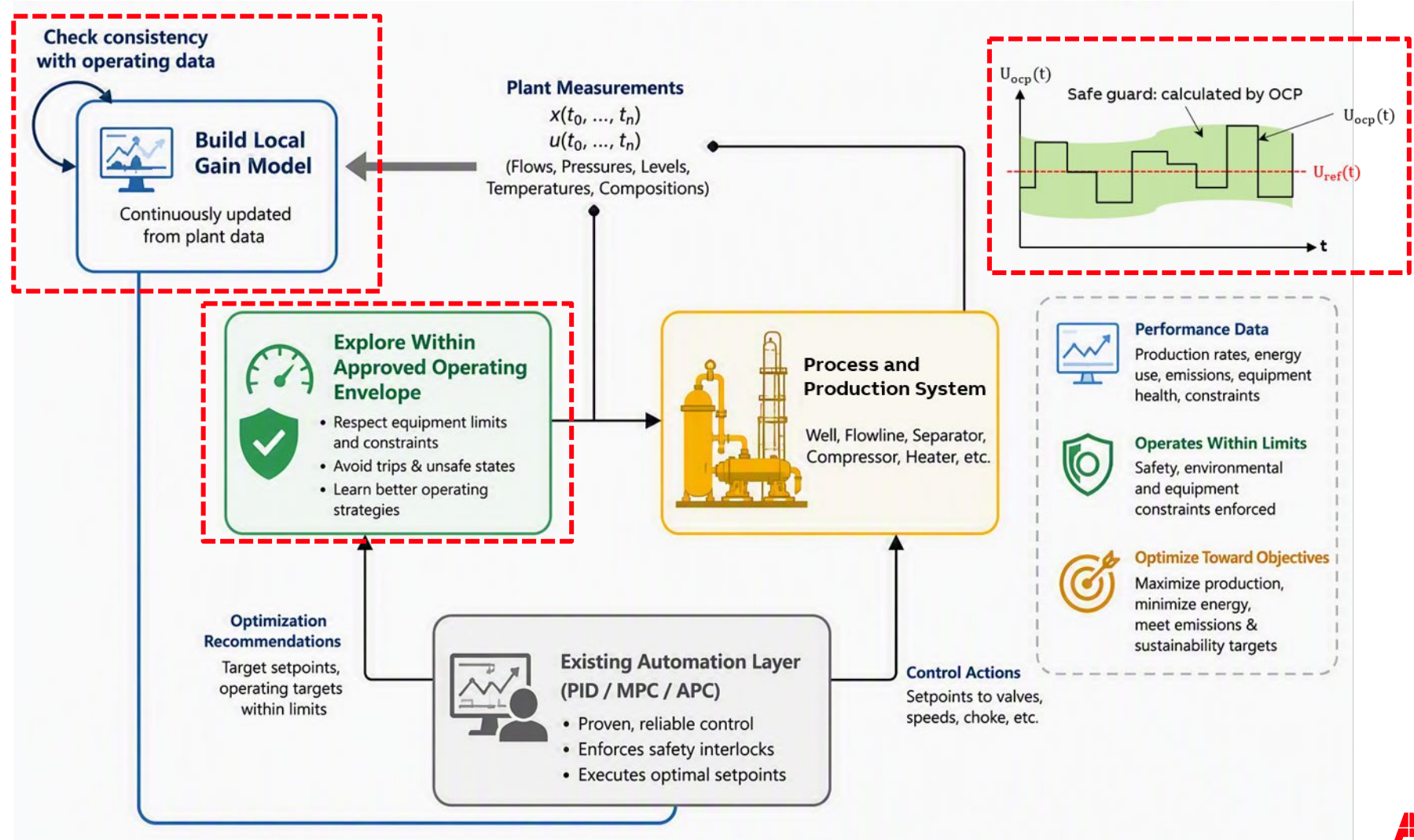
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Problem Formulation

How to use the explored data?

1. Build process models
2. Optimize operations
3. **Controller Tuning**
4. Train ML/AI models
5. Alarm rationalization?



Methodology

Linear form: LQR solution

For a linear system	$\dot{x}_t = Ax_t + Bu_t$
and LQR Objective	$\min_u \int_0^\infty (x_t^\top Q x_t + u_t^\top R u_t) dt$
The closed loop response:	$\dot{x} = Ax + Bu_{LQR} = (A - BK)x$
The quadratic Lyapunov function $V = x^\top P x$ guarantees system stability:	$\dot{V} = x^\top ((A - BK)^\top P + P(A - BK))x = -x^\top Q x < 0, \forall x \neq 0$

If the control input is perturbed:	$\dot{x} = Ax + B(u_{LQR} + \Delta u) = (A - BK)x + B\Delta u$
This perturbation is allowable if:	$\dot{V} = x^\top ((A - BK)^\top P + P(A - BK))x + 2x^\top PB\Delta u = -x^\top Q x + 2x^\top PB\Delta u < 0, \forall x \neq 0$
Exploration around LQR control action is safe if	$2x^\top PB\Delta u < x^\top Q x, \forall x \neq 0$

Solution method

- Generate random vector Δu
- Solve the optimization problem $\min_u \|u - (u_{LQR} + \Delta u)\|^2$, subject to $x^\top (A^\top P + PA)x + 2x^\top PBu < 0$

This optimization problem is always feasible because u_{LQR} satisfies the stability condition

Methodology

Formulation based on a 1D example

For a nonlinear form, we consider a Gaussian process to capture unmodelled dynamics:

$$\dot{x}_t = Ax_t + Bu_t + g(x)$$

mean $\mu_t(x)$ and
standard deviation $\sigma_t(x)$

Probabilistic Control Invariant Set

This set contains all states from which we can find a control action that keeps the system safe, even when the model is uncertain.

The uncertainty is learned using a **Gaussian Process (GP)**, so safety is guaranteed with **high probability** rather than absolute certainty.

$$\dot{V} + \text{uncertainty margin} + \lambda V \leq 0$$

Decay rate toward safety: How
fast the Lyapunov function
decreases

In simple words:

Even after accounting for the worst plausible model error, the Lyapunov function must still decrease.

This means the controller can keep driving the system toward the safe region.

Methodology

Formulation based on a 1D example

For a nonlinear form, we consider a Gaussian process to capture unmodelled dynamics:

$$\dot{\mathbf{x}}_t = \mathbf{A}\mathbf{x}_t + \mathbf{B}\mathbf{u}_t + \mathbf{g}(\mathbf{x})$$

Probabilistic Control Invariant Set

This set contains all states from which we can find a control action that keeps the system safe even when the model is uncertain.

The uncertainty is learned using a Gaussian process model with **probability** rather than absolute certainty.

The probabilistic control invariant set is the set of states from which a control action exists that guarantees Lyapunov-based safety despite GP model uncertainty, with confidence level

$$1 - \delta$$

In simple words:

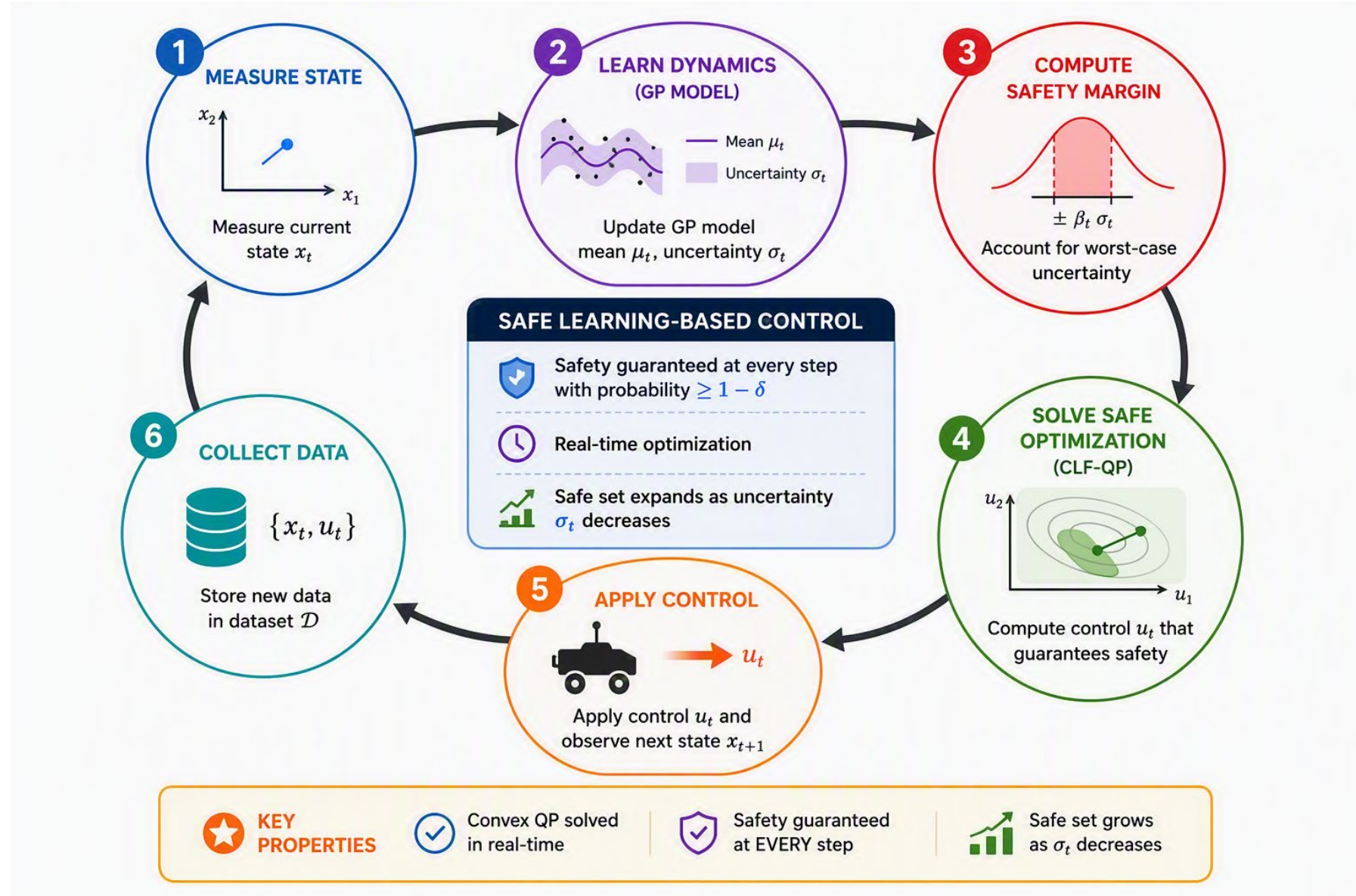
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<https://doi.org/10.48550/arXiv.2605.09772>

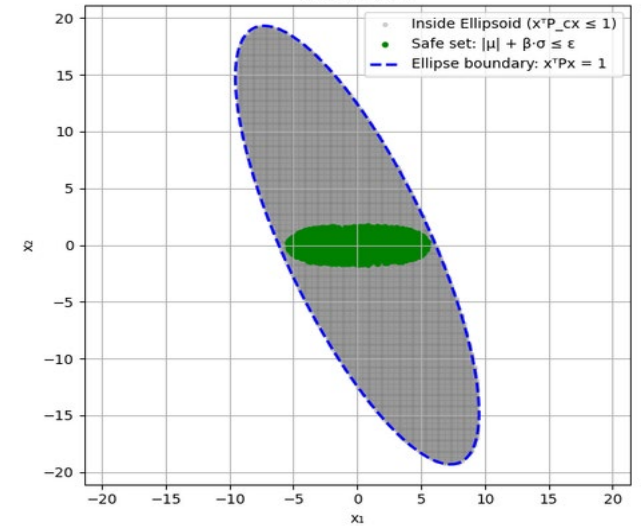
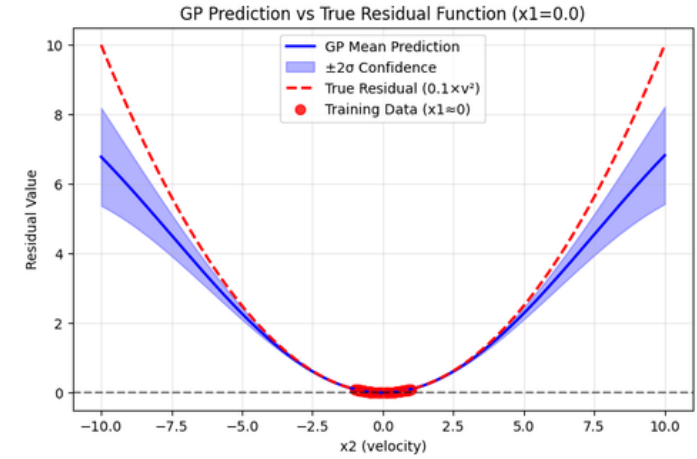
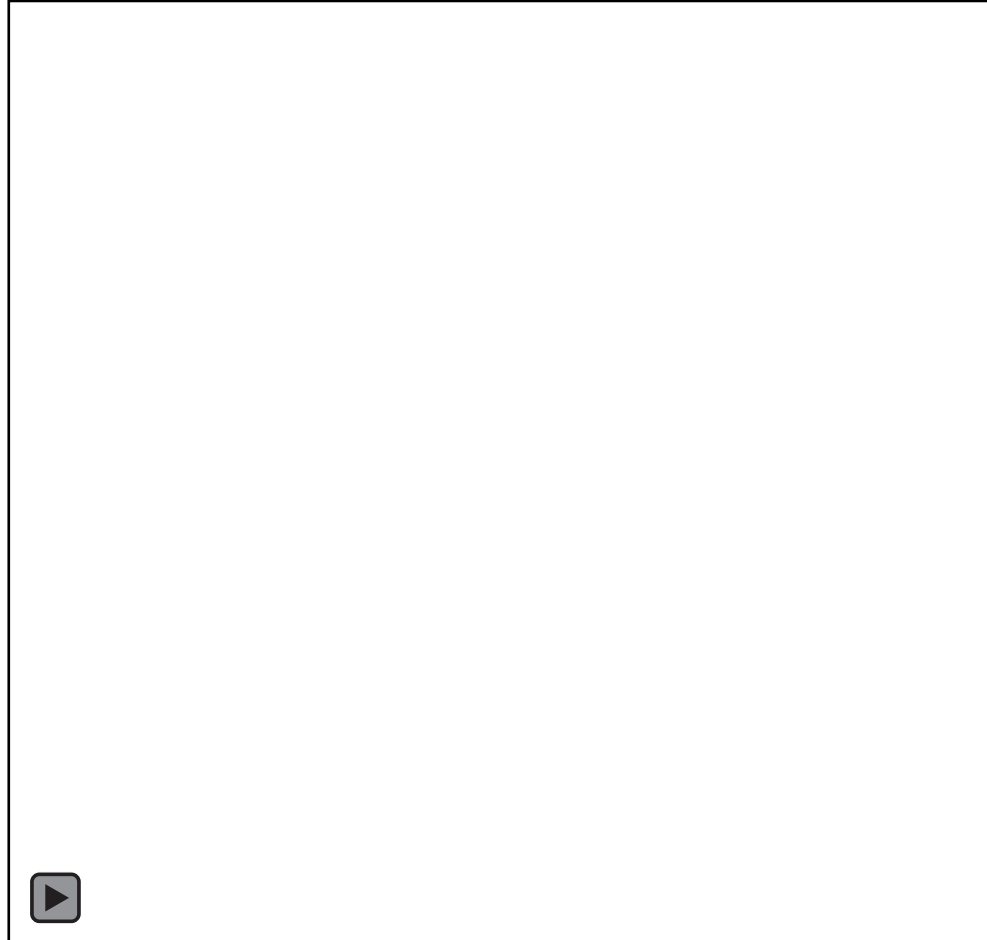
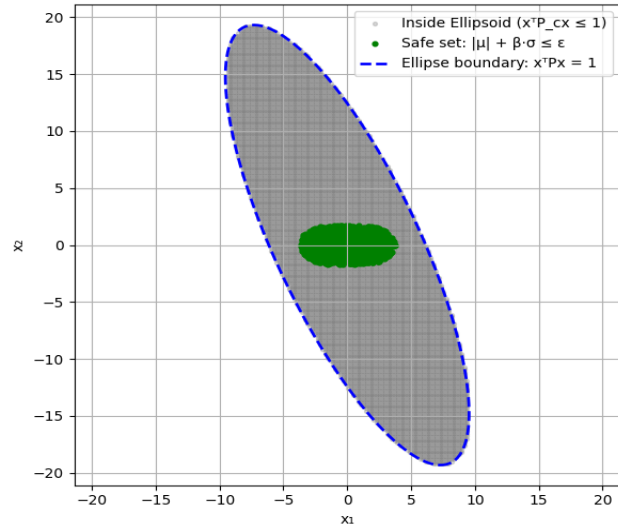
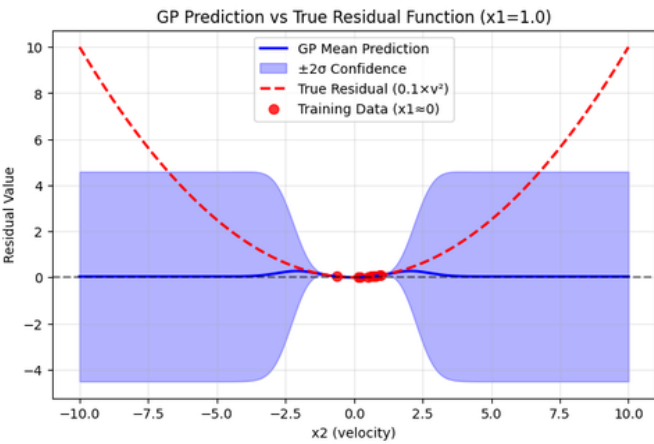
Methodology

Algorithm



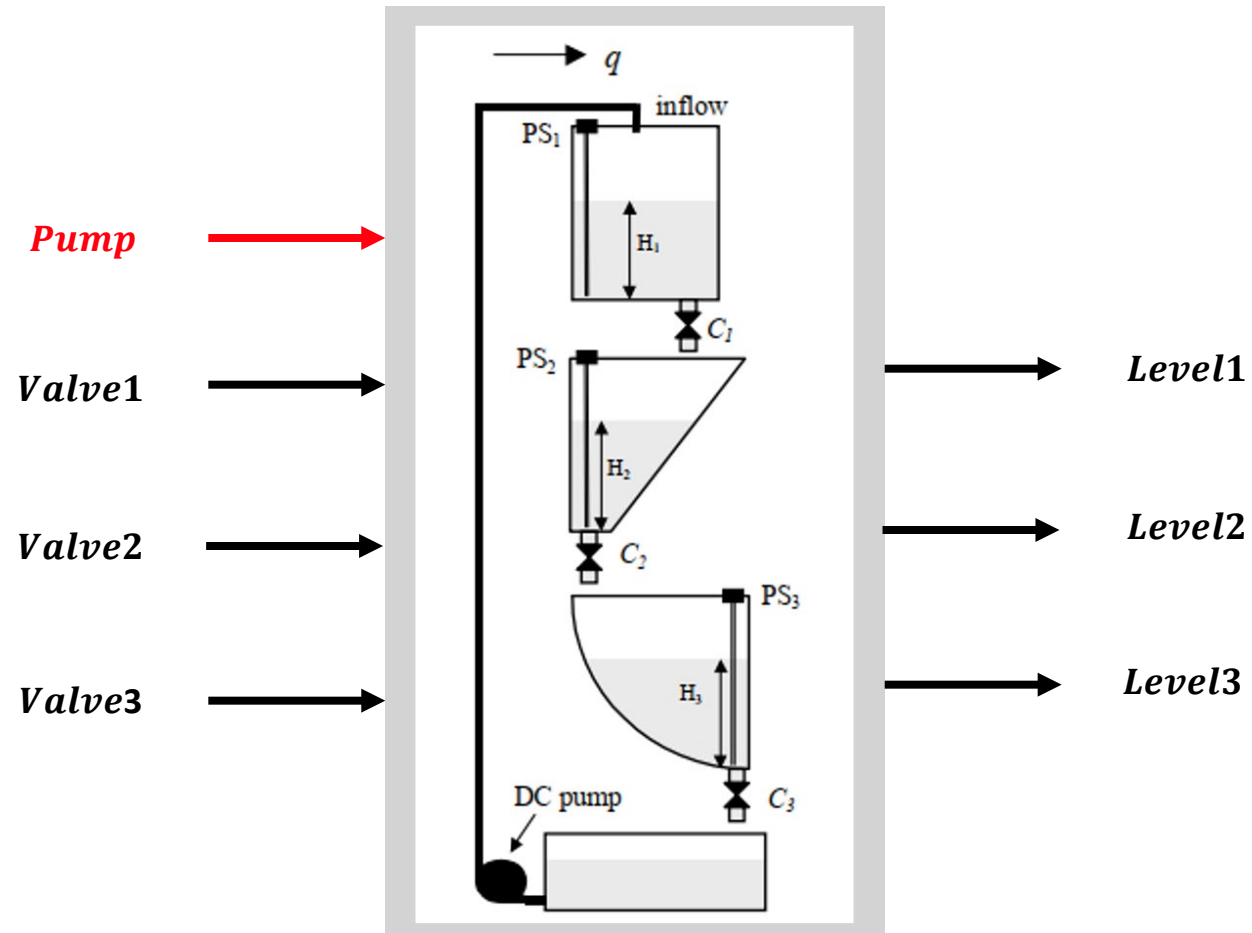
Methodology

1D example: $\dot{v} = -2v + v^2 + u$



Methodology

Benchmark example of a 3×3 system

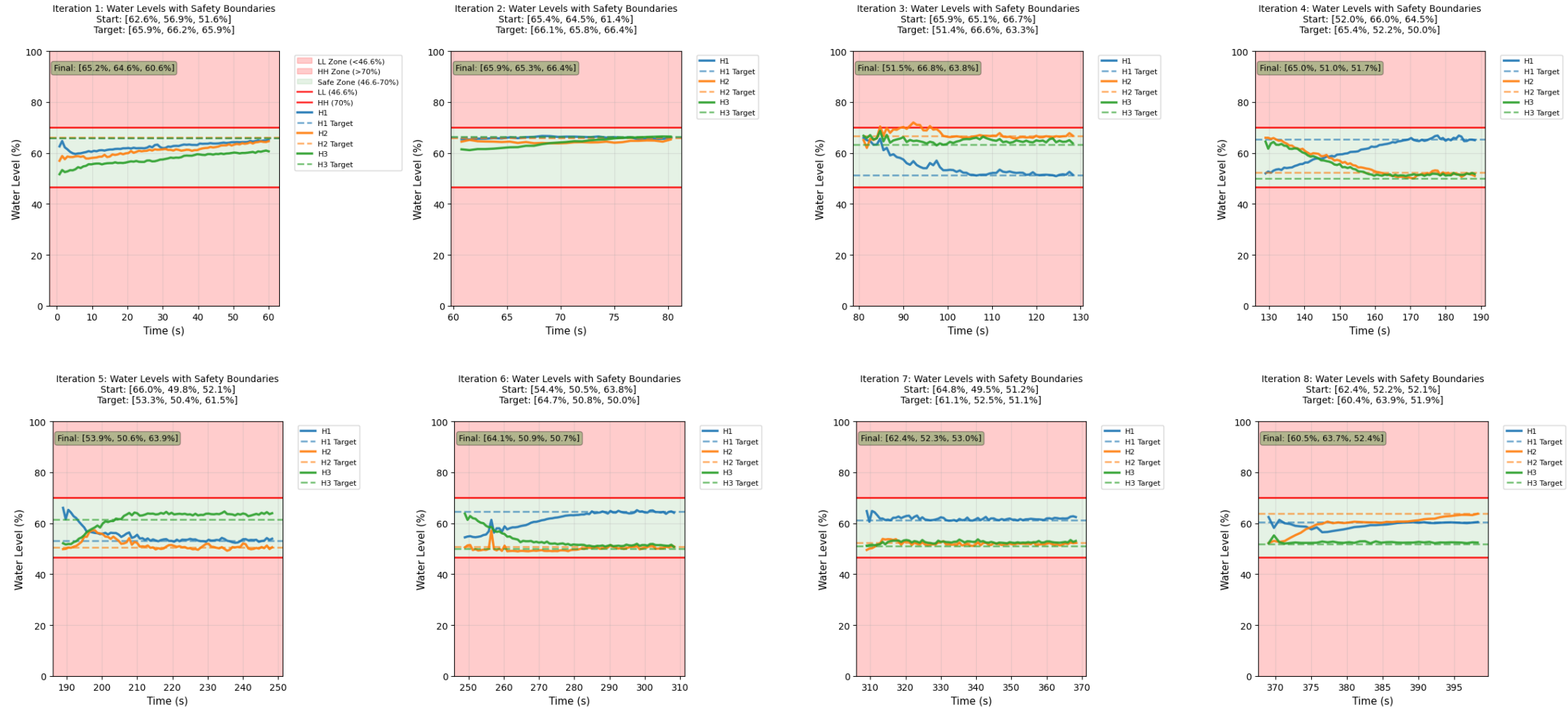


Methodology



Methodology

Benchmark example of a 3 × 3 system

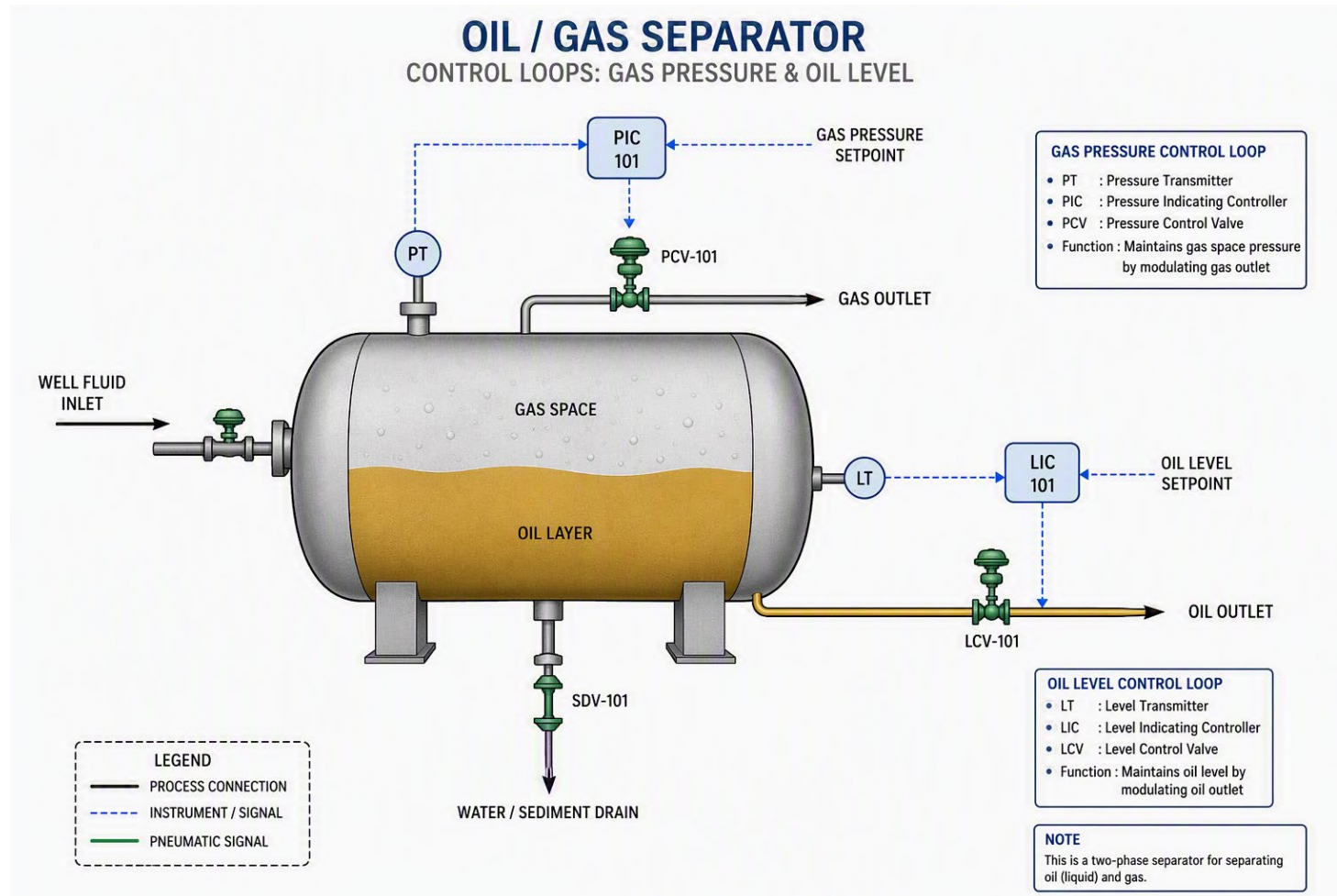


TWO-PHASE SEPARATOR

- Online Controller Tuning

Safe Exploration → Exploitation

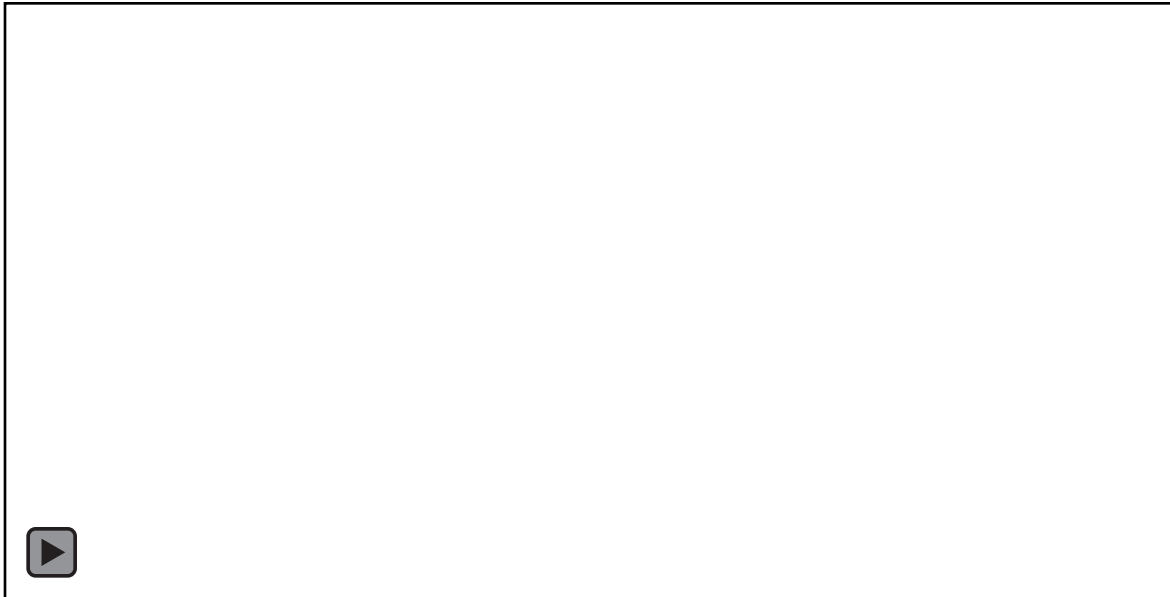
Online Controller Tuning



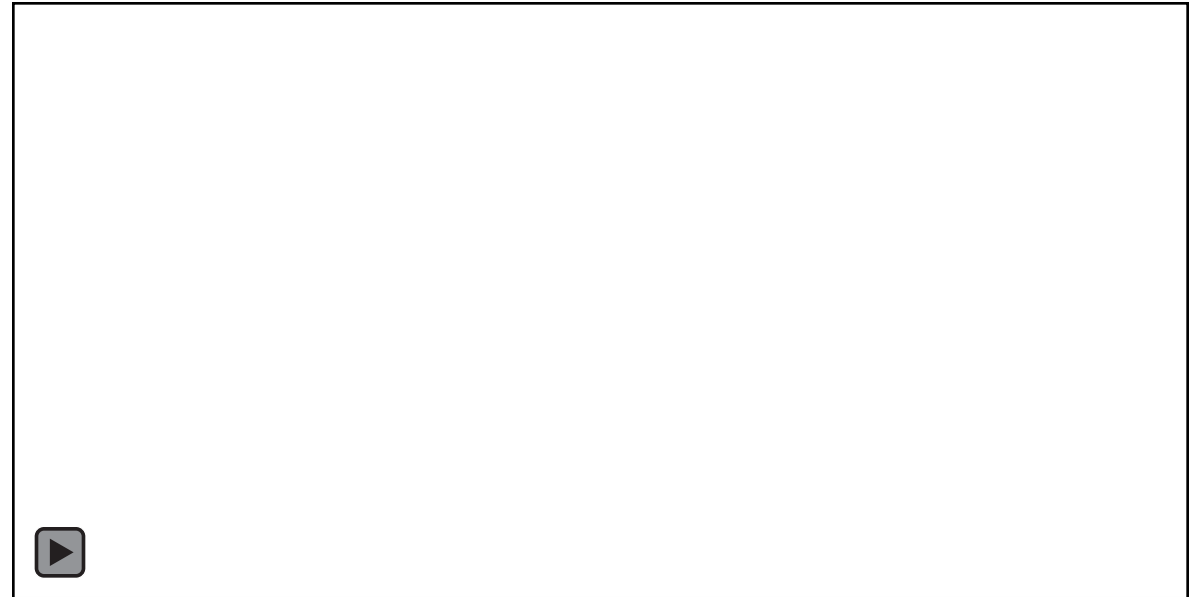
Safe Exploration → Exploitation

Online Controller Tuning

Oil level



Gas pressure



Conclusion

- Online safe experimentation
- Stability guarantee during operation
- Constraint guarantee during operation
- Space for local controller tuning thanks to the exploration data
- No engineering work during operation (fully autonomous system)
- Fast training time for machine learning approaches like RL (Offline, augmented RL)

ABB

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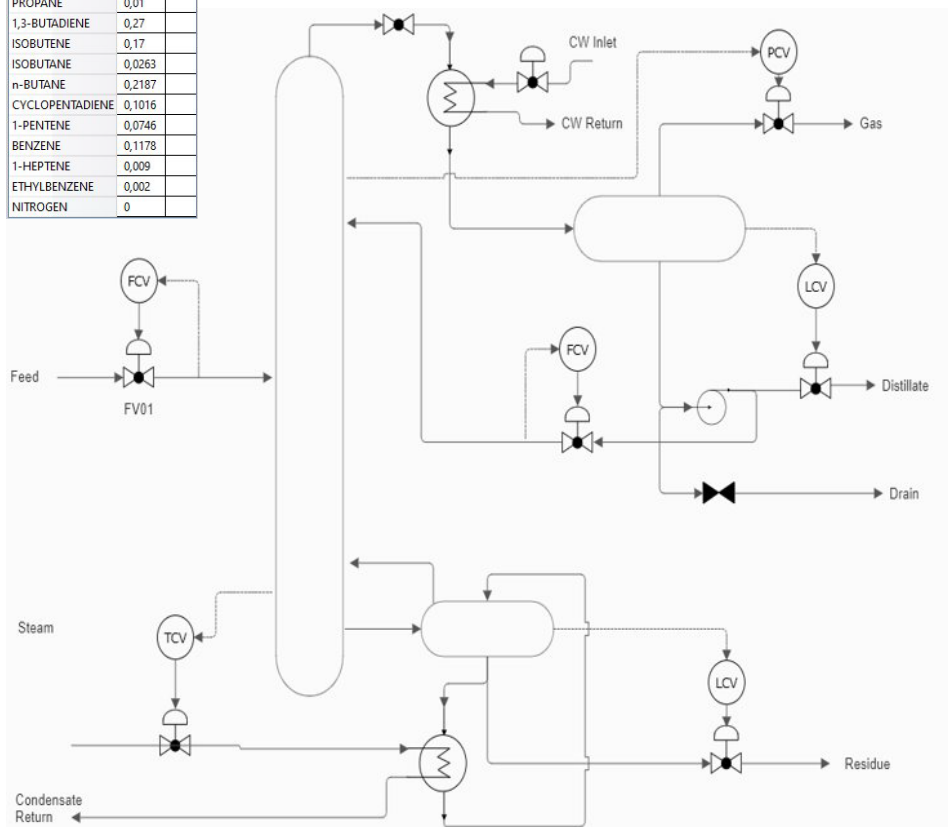
DISTILLATION COLUMN

- Offline Reinforcement Learning

Safe Exploration → Exploitation

- Offline Reinforcement Learning

	col [0]	
WATER	0	
HYDROGEN	0	
METHANE	0	
PROPANE	0,01	
1,3-BUTADIENE	0,27	
ISOBUTENE	0,17	
ISOBUTANE	0,0263	
n-BUTANE	0,2187	
CYCLOPENTADIENE	0,1016	
1-PENTENE	0,0746	
BENZENE	0,1178	
1-HEPTENE	0,009	
ETHYLBENZENE	0,002	
NITROGEN	0	



Product quality target:

- Butadiene composition [**>0.3 gram/gram**]
- Benzene composition [**>0.4 gram/gram**]

Actions:

- Reflux flow control (FC03) setpoint [30000-100000] kg/h
- Steam Flow control (FC05_A) setpoint [0-23000] kg/h
- Vent Flow control (FC04_A) setpoint [0-5800]

External input: Feed flow (FC01) setpoint (55000kg/h) [30000-60000]

Goal: Maximize profit while ensuring product quality is above target.

Observations:

- Reflux Level (%)
- Reboiler Level (%)
- Distillate Flow (kg/sec)
- Residue Flow (kg/sec)
- Feed Flow (kg/sec)
- Top Temperature (degC)
- Bottom Temperature (degC)
- Top Pressure (bar)
- Bottom Pressure (bar)
- But, Benz composition (top and bottom)

Safe Exploration → Exploitation

- Offline Reinforcement Learning

$$\text{Revenue} = \text{Cost}_{\text{Butadiene}} * \text{Flow}_{\text{Distillate}} * \text{Comp}_{\text{Butadiene_Distillate}} + \text{Cost}_{\text{Benzene}} * \text{Flow}_{\text{Residue}} * \text{Comp}_{\text{Benzene_Residue}}$$

$$\text{Cost} = \text{Cost}_{\text{Feed}} * \text{Flow}_{\text{Feed}} + \text{Cost}_{\text{Steam}} * \text{Flow}_{\text{Steam}}$$

$$\text{Waste} = \text{Cost}_{\text{Butadiene}} * \text{Flow}_{\text{Vent}} * \text{Comp}_{\text{Butadiene_Vent}} + \text{Cost}_{\text{Benzene}} * \text{Flow}_{\text{Vent}} * \text{Comp}_{\text{Benzene_Vent}}$$

$$\text{Profit} = \text{Revenue} - \text{Cost} - \text{Waste}$$

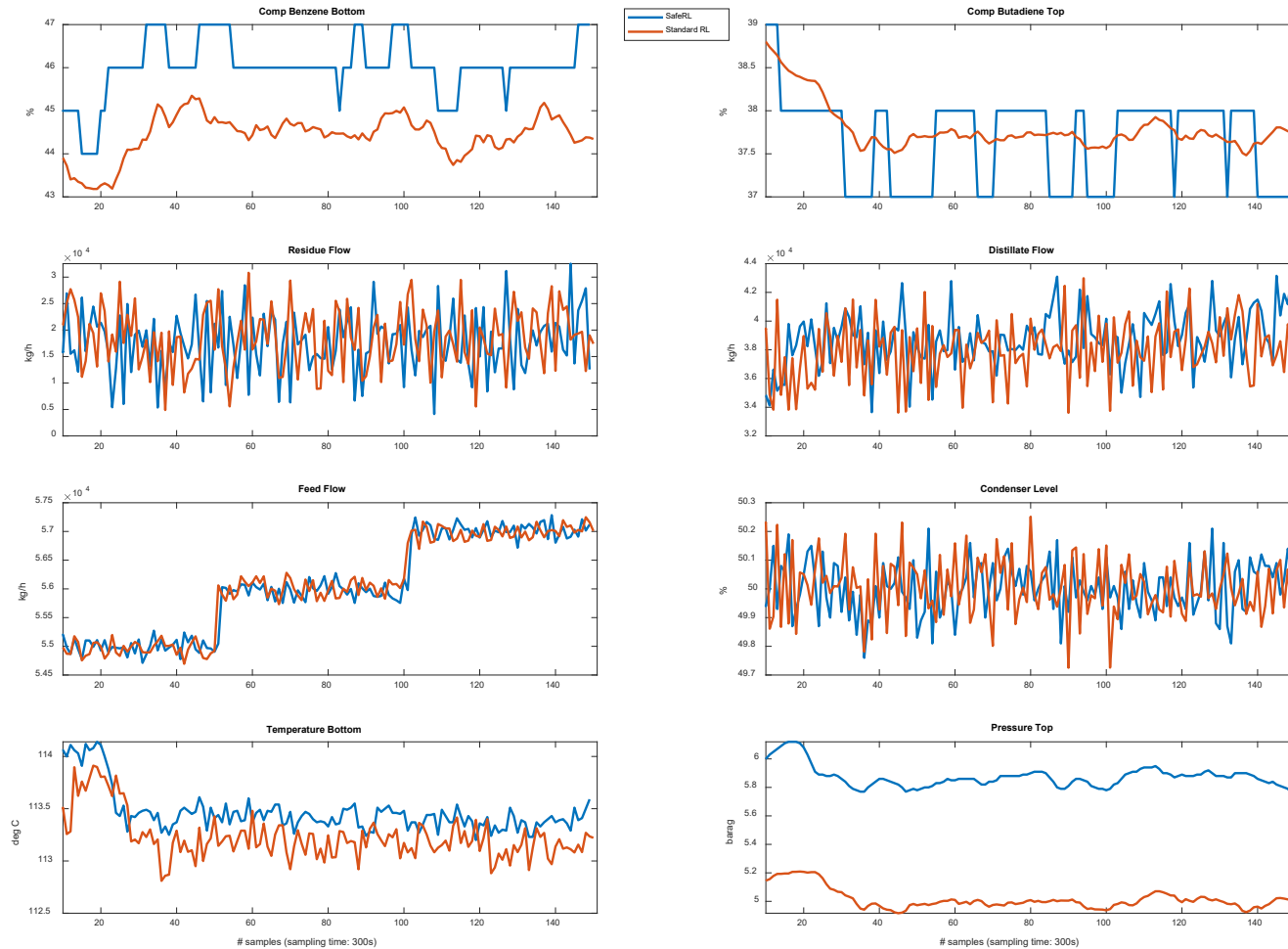
$$\text{Quality}_{\text{Penalty}} = (\text{Butadiene}_{\text{Target}} - \text{Butadiene}_{\text{Purity}} \text{ if } \text{Butadiene}_{\text{Purity}} < \text{Butadiene}_{\text{Target}} \text{ else } 0) \\ + (\text{Benzene}_{\text{Target}} - \text{Benzene}_{\text{Purity}} \text{ if } \text{Benzene}_{\text{Purity}} < \text{Benzene}_{\text{Target}} \text{ else } 0)$$

$$\text{Flow}_{\text{penalty}} = (\exp(0.5 - \text{Flow}_{\text{Distillate}}) \text{ if } \text{Flow}_{\text{Distillate}} < 0.5 \text{ else } 0) + (\exp(0.5 - \text{Flow}_{\text{Residue}}) \text{ if } \text{Flow}_{\text{Residue}} < 0.5 \text{ else } 0)$$

$$\text{Reward} = W_{\text{Profit}} * \text{Profit} - W_{\text{Quality}} * \text{Quality}_{\text{Penalty}} - W_{\text{flow}} * \text{Flow}_{\text{Penalty}}$$

Safe Exploration → Exploitation

- Offline Reinforcement Learning



Control Strategy

- Ranges

Variable	Min	Max	Nominal	Unit	Action Min	Action Max	Comment	Normalized Nominal	Normalized Min	Normalized Max
Feed Flow Rate (FT01)	0	85000	55000	Kg/h	52250	57750	5% deviation	0.647058824	0.614705882	0.679411765
Reflux Flow (FT03)	0	150000	43000	Kg/h	34400	51600	20% variation	0.286666667	0.229333333	0.344
Vapor Flow (FT04)	0	9000	2309.12	Kg/h	1847.293	2770.9392	20% variation	0.256568444	0.205254756	0.307882133
Steam Flow (FT05)	0	25000	11396.1	Kg/h	9116.9	13675.35	20% variation	0.455845	0.364676	0.547014
Bottom Flow (FT06)	0	60000	23800	Kg/h	19039.99	28559.988	20% variation	0.3966665	0.3173332	0.4759998
Distillate Flow (FT09)	0	155000	28896.6	Kg/h				0.186429981		
Butadiene Composition (Distillate)	0	1	0.86045	mol/mol				0.860446		
Benzene Composition (Distillate)	0	1	0	mol/mol				0		
Butadiene Composition (Bottom)	0	1	5E-06	mol/mol				0.000005		
Benzene Composition (Bottom)	0	1	0.66048	mol/mol				0.660483		
Column Top Temperature	0	150	47.12	degC				0.314133333		
Column Bottom Temperature	0	150	106.26	degC				0.7084		
Column Top Pressure	0	9	3.68	bar				0.408888889		
Column Bottom Pressure	0	9	3.92	bar				0.435555556		
Reboiler Shell Level	0	100	50	%				0.5		
Reflux Drum Level	0	100	50	%				0.5		