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Hybrid Modelling and Optimisation Framework for Plant-Wide Real-Time Applications

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The Spiro Team

The Managing Director and founder of Spiro, with 35 years of experience in APC and optimisation, has led over 40 APC projects and developed several commercial software products, including APC, model identification, PID tuning, and RTO.

Dr Patrick Thorpe

Senior Consultant with five decades of experience in industrial process control and optimisation, and a recognised authority in ethylene process APC. Along with Dr Thorpe, Doug was a co-founder of Aptitude, a technology startup sold to IPCOS.

Doug Nicholson

Process modelling and control specialist with extensive commercial software development expertise and a deep understanding of linear algebra and control theory. Shabroz is an IIT graduate and is the principal architect behind Spiro’s products.

Shabroz Gill

Chemical Engineer with 20 years of experience in APC and optimisation across refining and petrochemicals, including more than 10 dynamic optimisation projects.

Dario Ferraro

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Real Time Optimisation (RTO) Requirements

Definition: Real-Time Optimisation (RTO) combines a calibrated process model with an optimiser to continuously drive a process to the best feasible operating point. A well-designed and well-maintained RTO can achieve significant benefits.*

For an RTO project to justify the investment, it should:

- Increase operating margins and achieve a quick return on investment.
- Deliver capabilities beyond what linear model predictive control can achieve.

But RTO can be:

- Complex and costly to build, implement, and maintain.*
- Vulnerable to downtime and low availability.

Requirement – to develop an RTO solution that achieves the same benefits but with:

- Reduced cost.
- Simplified maintenance.
- High availability.
- Support for multiple use cases (open-loop and closed-loop RTO, ad-hoc optimisation and what-if studies).

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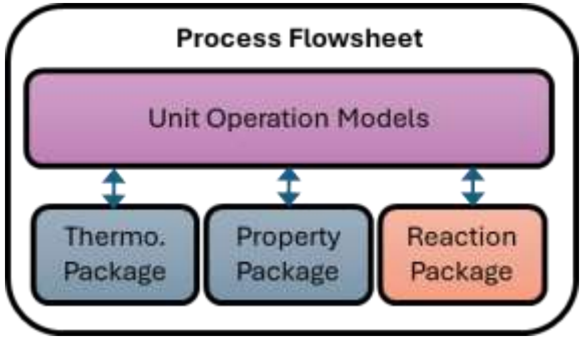
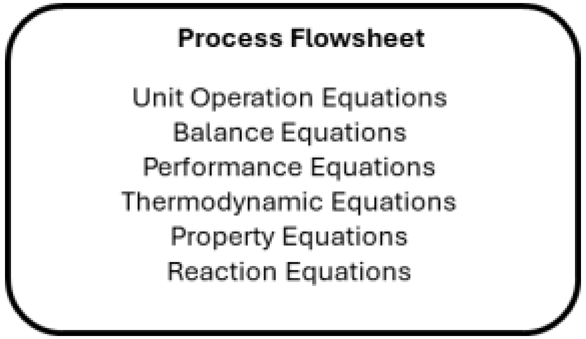
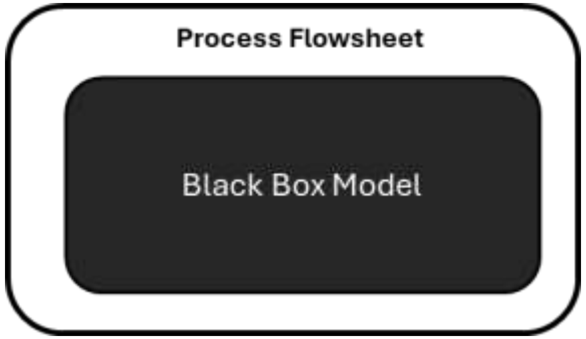
*Reference: Darby et al., 2011

Modelling Methods for Real-Time Optimisation

Sequential Modular Simulation		
• Solves each flowsheet block in sequence. • Flowsheets can be prototyped and run relatively quickly. • Good diagnostics, easy to isolate errors.	• The model input-output structure is fixed by the design and use case. • Optimisation solutions may take a long time to converge. • Recycle streams and design specifications are solved iteratively.	
Equation Oriented Simulation		
• Collects all model equations and solves them simultaneously. • The model input-output structure can be easily modified according to context. • Optimisation solutions can run quickly on a converged model.	• Higher model-building effort and skills needed. • Diagnostics and debugging can be difficult. • Solutions are sensitive to initial conditions and scaling. • Requires a robust nonlinear solver.	
AI Surrogate Models		
• Fast execution once the model is trained. • Captures complex non-linearities. • Models can be differentiable and support gradient-based optimisation.	• Poor extrapolation outside the training set. • Hard to enforce balance constraints. • Explainability and validation are challenging. • Extensive data required for training. • Require high maintenance (frequent re-training) due to data drift.	

Hybrid Modelling and Optimisation Framework

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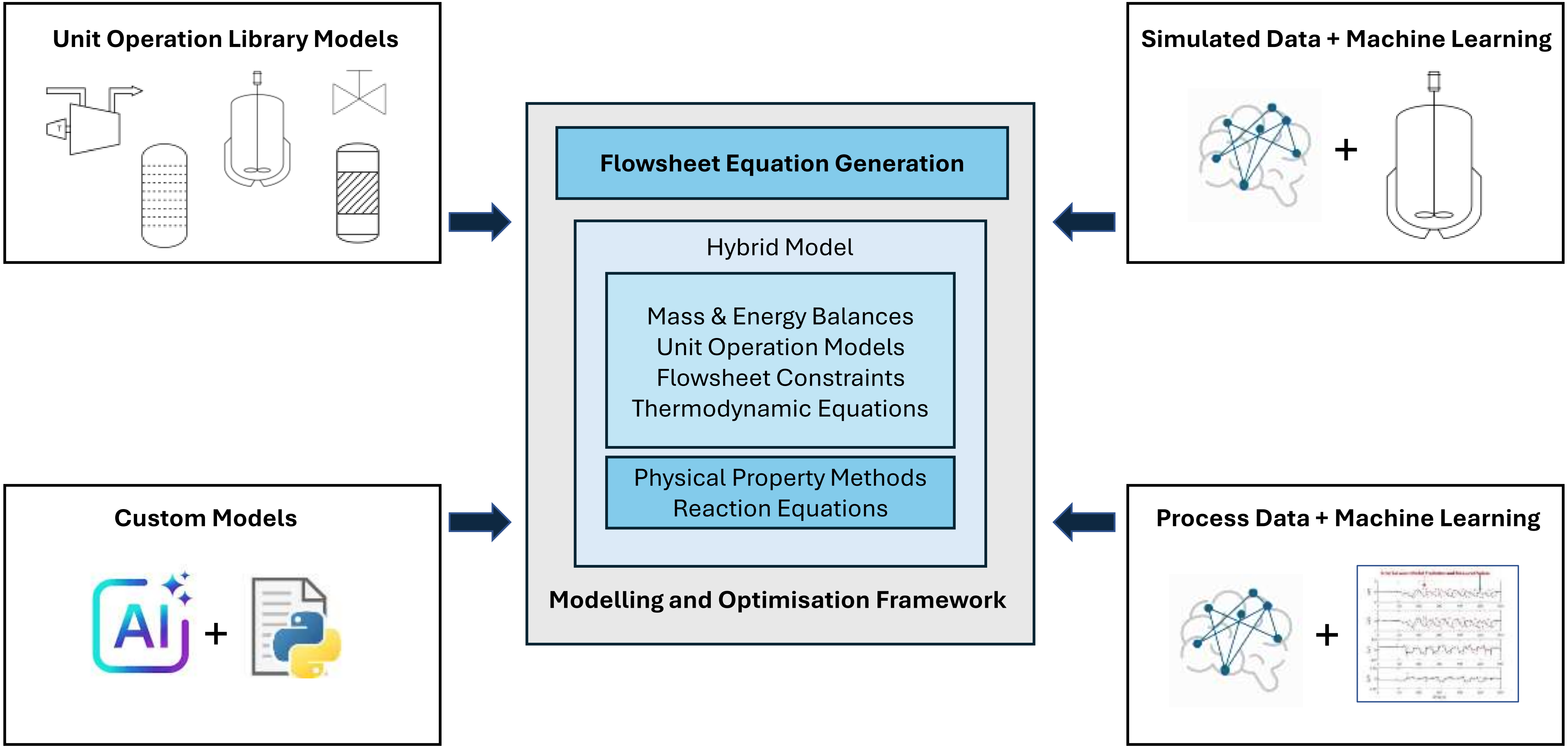
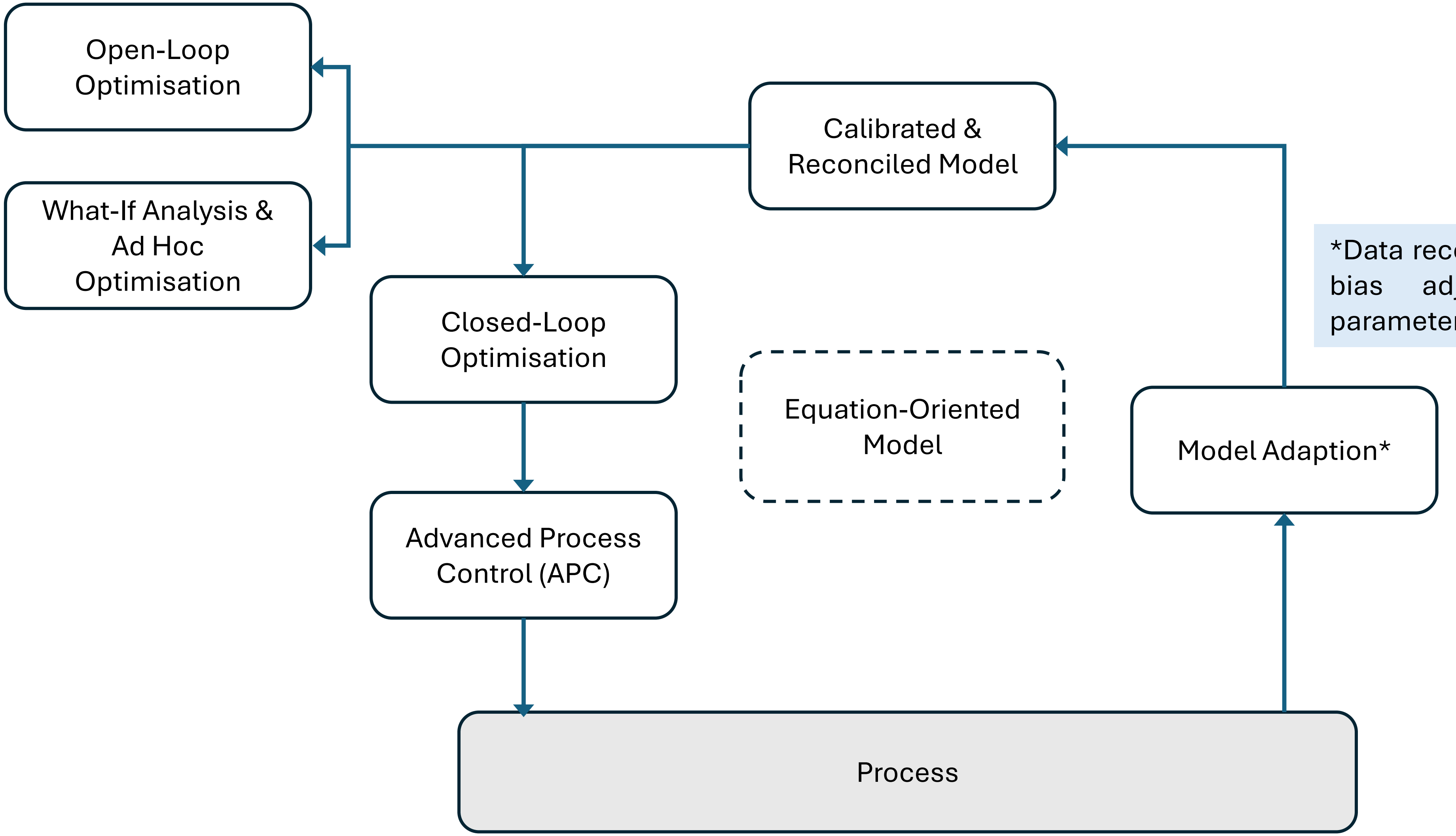


The RTO Execution Cycle

Each solution step utilises the same Equation-Oriented model, but with a different set of constraint conditions and degrees of freedom.



*Data reconciliation (measurement bias adjustment) and model parameter estimation.

Degrees of Freedom, Context & Model Validation

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Offline Application Builder

Degrees of freedom are calculated at the flowsheet and unit operation level to facilitate model diagnostics.

Contexts are used to manage the degrees of freedom for each solution step (initialise, simulate, estimate, optimise, etc.).

EthyleneDemo

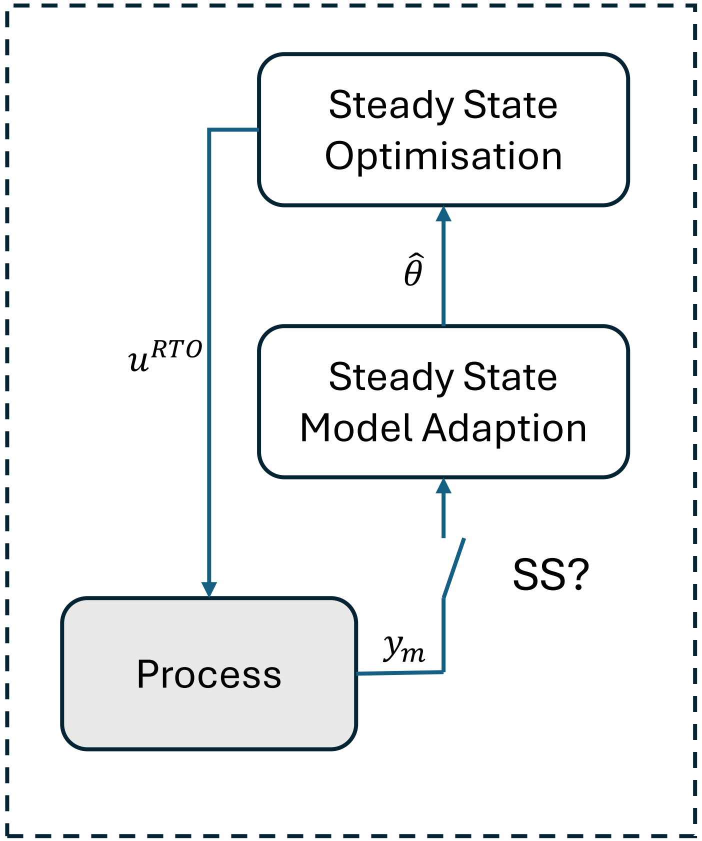
- + Feed_and_Furnaces (0)
- + CGC_and_Deprop (0)
- – Cold_Section (1)
  - Cooler_200 (0)
  - Cold_box_separator2 (0)
  - Cooler_206 (0)
  - Cold_box_separator3 (0)
  - Cold_box_valve1 (0)
  - Cooler_196 (1)
  - Cold_box_separator1 (0)
  - Sep_2_liq_valve (0)
  - Sep_1_liq_valve (0)
  - Sep_3_liq_valve (0)
  - Cold_box_valve2 (0)
  - Cold_box_valve3 (0)
  - C2s_ohd_sensor (0)
  - Fcc_c2 (0)
  - C2s (0)
  - Deethaniser2 (0)
  - Deeth2_feed_sensor (0)
  - Deeth2_feed_pump (0)
  - Demethanizer (0)
  - Demeth_feed_sensor (0)
  - Demeth_ohd_sensor (0)
  - Deeth2_ohd_sensor (0)
  - Deeth2_btm_sensor (0)

CONTEXTS | LOG

Name	Var Value	Initial Value	Context	Is Measured
			MV OR CV	
Feed_and_Furnaces.f4.sor	0.5	0.5	MV	☑
Feed_and_Furnaces.f5.cot	1150	1150	MV	☑
Feed_and_Furnaces.f1.cot	1094.15	1094.15	MV	☑
Feed_and_Furnaces.f3.sor	0.5	0.5	MV	☑
Feed_and_Furnaces.f5.sor	0.5	0.5	MV	☑
Feed_and_Furnaces.f1.sor	0.5	0.5	MV	☑
Feed_and_Furnaces.C2_split.split_fraction_1	0.4	0.4	MV	☐
Feed_and_Furnaces.f2.cot	1094.15	1094.15	MV	☑
Feed_and_Furnaces.c3plus_split.split_fraction_2	0.4	0.4	MV	☐
Feed_and_Furnaces.f2.sor	0.5	0.5	MV	☑
Feed_and_Furnaces.c3plus_split.split_fraction_3	0.4	0.4	MV	☐
Feed_and_Furnaces.C2_split.split_fraction_2	0.4	0.4	MV	☐
Feed_and_Furnaces.f4.cot	1150	1150	MV	☑
Feed_and_Furnaces.f3.cot	1150	1150	MV	☑
Feed_and_Furnaces.furnace_custom_logic.F4_F5_FlowDiff	-3.0714256793765386e-33		CV	☐
Feed_and_Furnaces.f2.ethane_conversion	69.42024283812121		CV	☐
Feed_and_Furnaces.f4.inlet.flow_mol	305.35436443734324	285	CV	☑
Feed_and_Furnaces.f4.butane_conversion	74.30750029756402		CV	☐

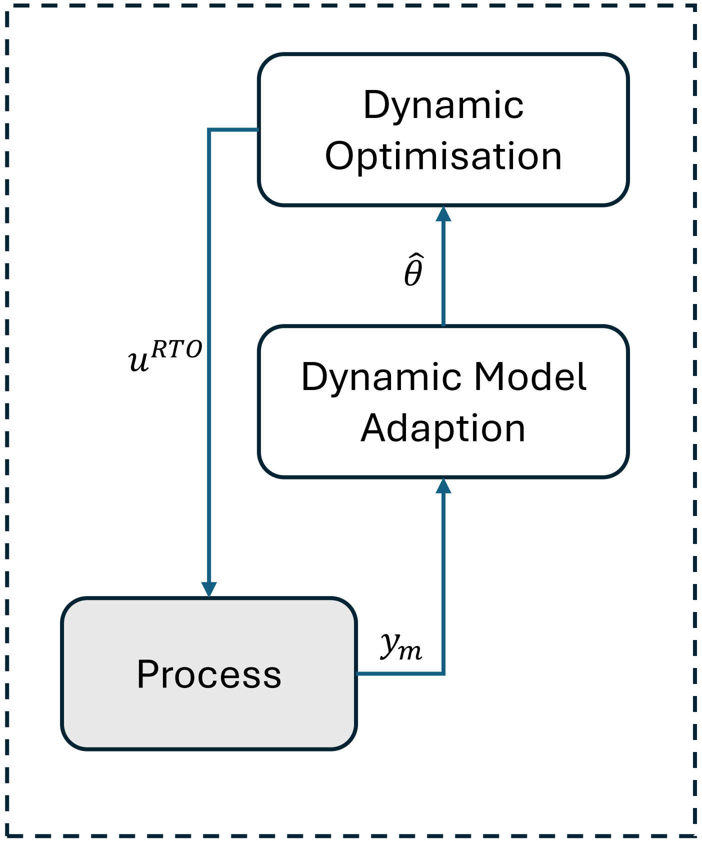
Steady State vs Dynamic vs Hybrid RTO

Steady State RTO



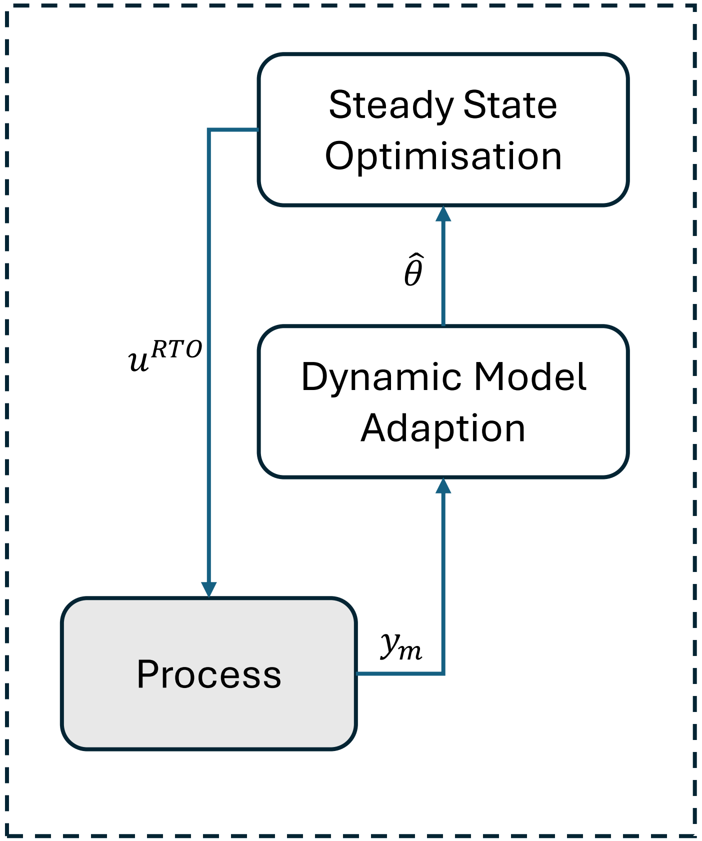
Steady state model adaption with steady state optimisation.

Dynamic RTO



Dynamic model adaption with dynamic optimisation.

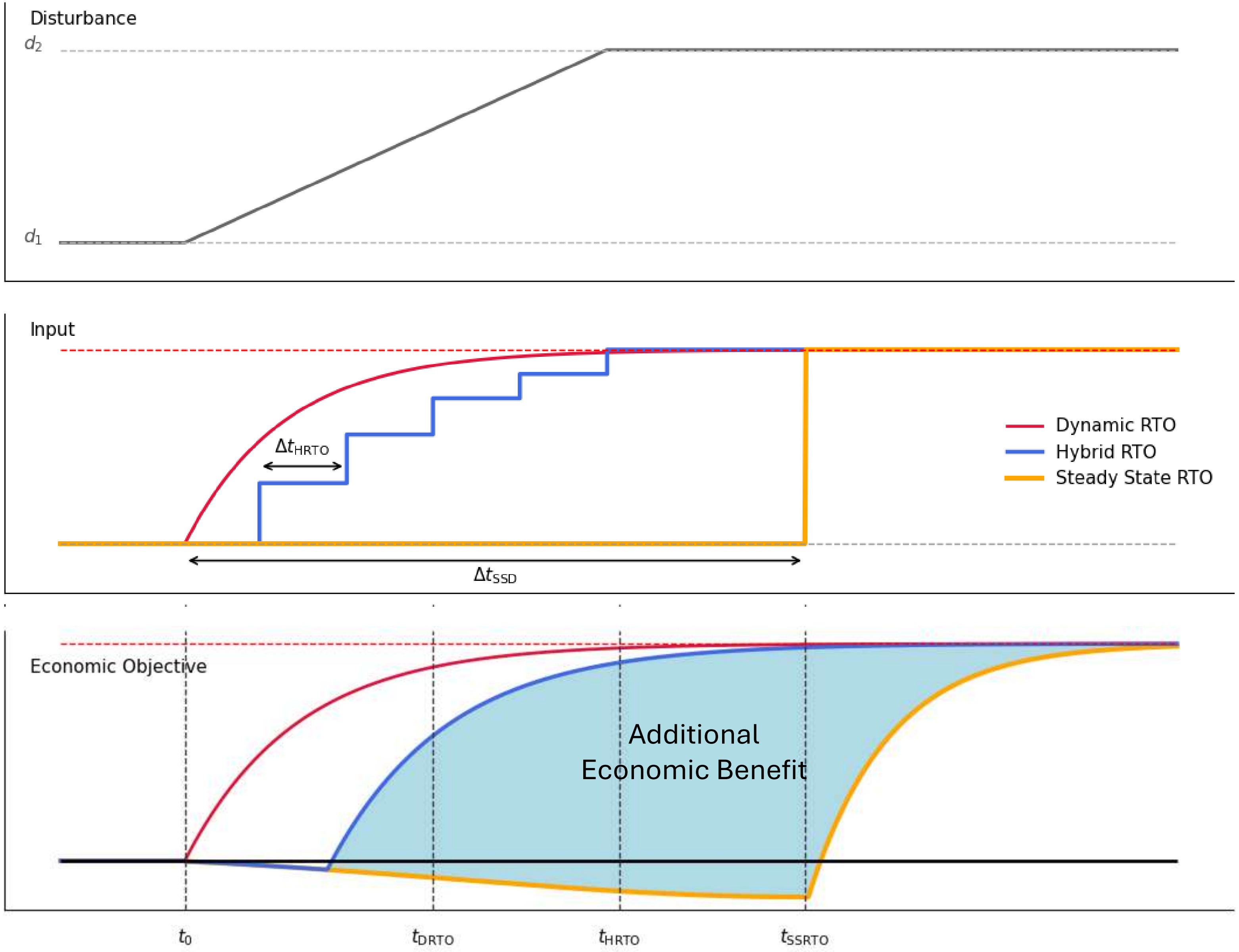
Hybrid RTO



Dynamic model adaption with steady state optimisation.

Reference: Krishnamoorthy, Foss and Skogestad, 2018

Steady State vs Dynamic vs Hybrid RTO



Ramp Disturbance

RTO Closed Loop Response

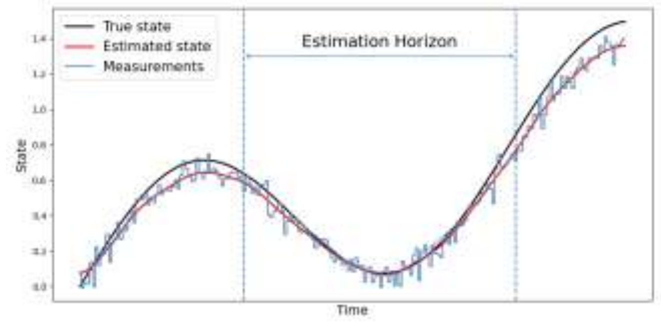
Process Response (Objective Function)

Dynamic Model Adaption

Moving Horizon Estimation

Reference: Hedengren and Eaton, 2017

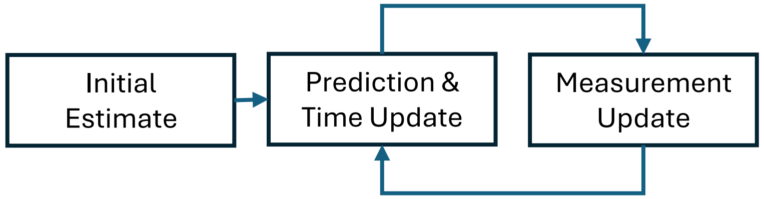
- Solves a dynamic optimisation problem at each sampling instant.
- Includes constraints.
- Computationally intensive.
- Arrival cost estimation adds additional complexity.
- Differential–algebraic (DAE) or discrete state space dynamic model.



Nonlinear Kalman Filter

Reference: Krishnamoorthy, Foss and Skogestad, 2018

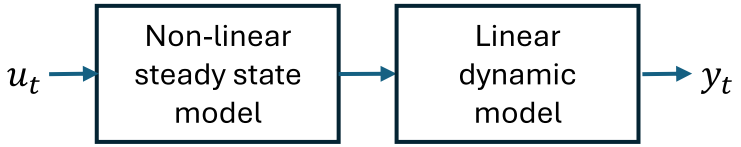
- Simple to implement and computationally fast.
- Does not need to solve a nonlinear optimisation problem online.
- Tuning can be complex.
- Doesn’t handle constraints directly.
- Discrete state-space dynamic model.



Hammerstein Dynamic Model

Reference: Delou et al, 2021

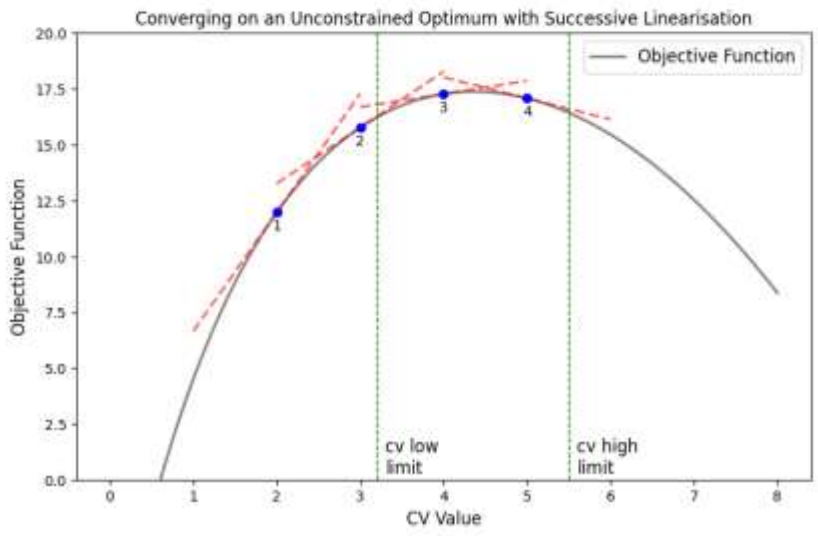
- Combines a non-linear steady state model with identified plant dynamics.
- Uses a modified Kalman filter formulation, denoted Hammerstein EKF.
- Ensures consistency between APC and RTO dynamics.
- ARX dynamic model.



Steady State Optimisation with a Nonlinear Model

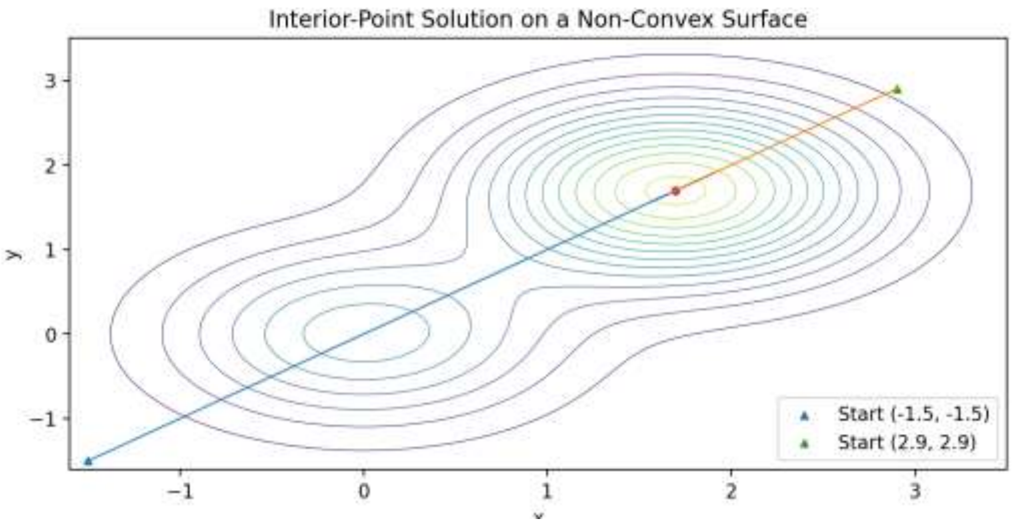
Successive Linearisation

- Effective for convex or mildly nonlinear problems.
- Quadratic objective function – deterministic and fast solution.
- Can be deployed as closed-loop RTO (hill climbing).
- Linearised models can be reused for planning and APC.
- Requires a carefully defined trust region.
- The open-loop solution is valid only near the linearisation point – makes commissioning difficult.
- Not suitable for what-if studies and ad-hoc optimisation.

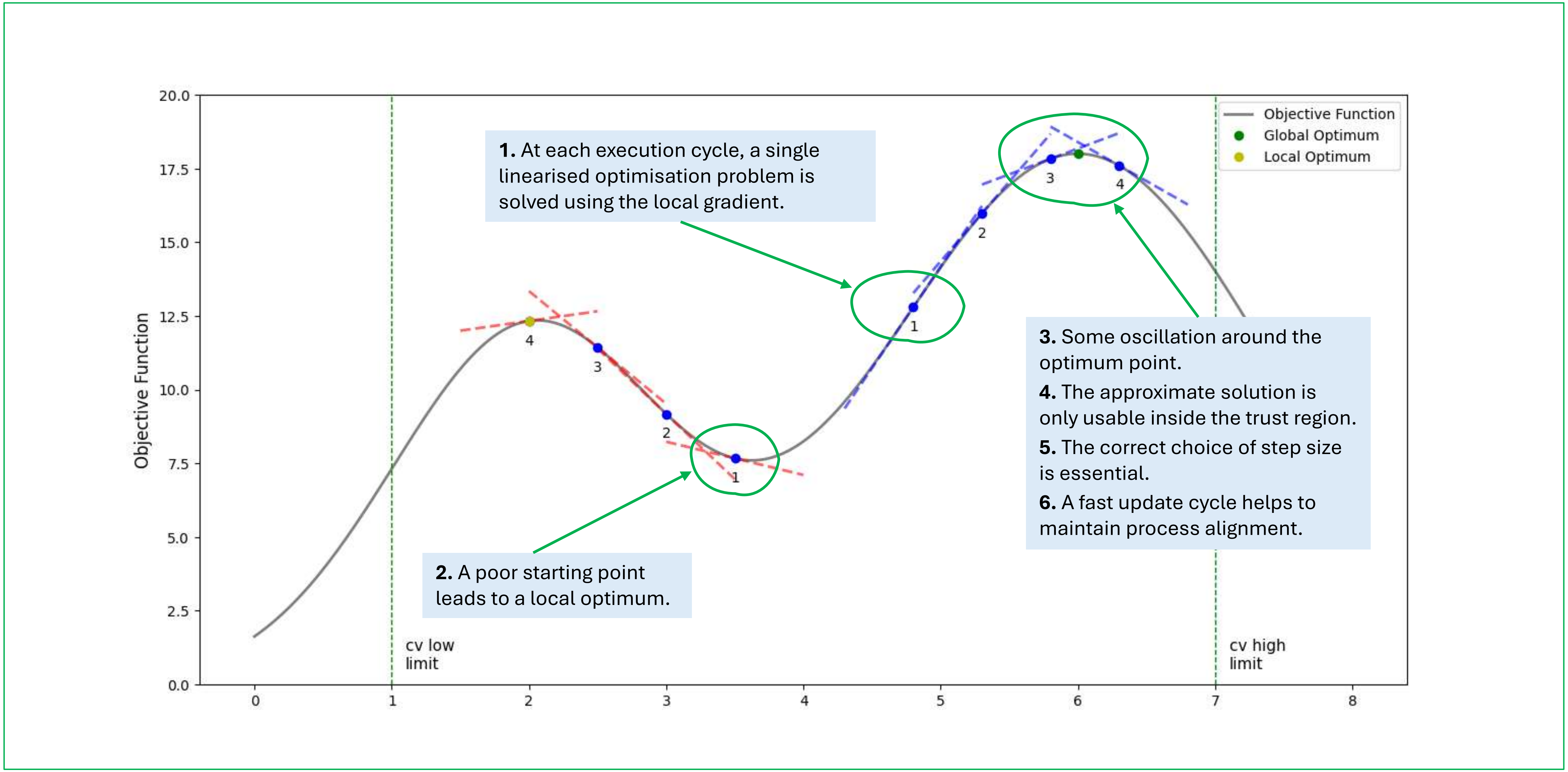


Non-linear Optimisation

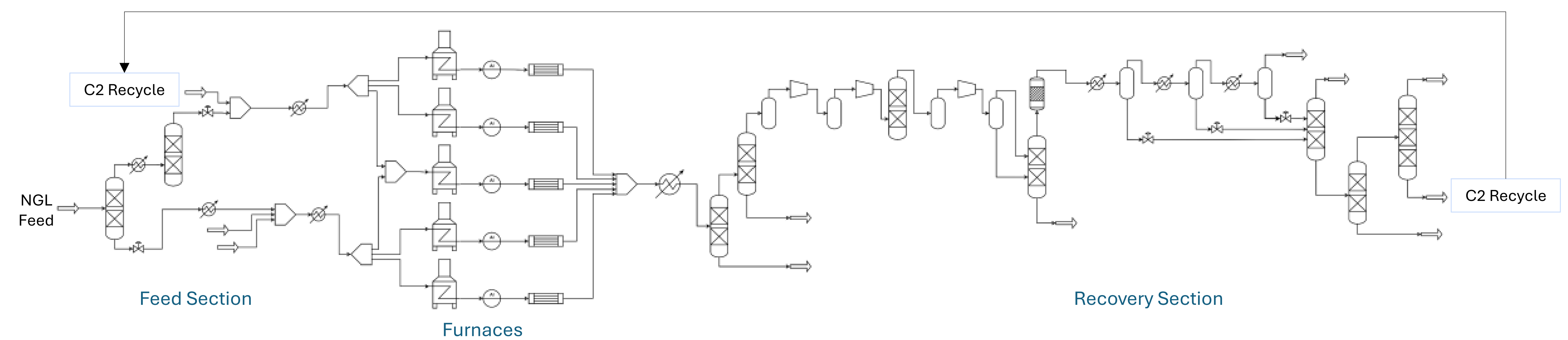
- Applicable to convex and non-convex optimisation problems.
- Supports closed-loop and open-loop RTO, as well as what-if analysis and ad-hoc optimisation.
- Global optimum solution if properly initialised & constrained.
- Two-stage commissioning (open-loop → closed-loop) builds confidence & acceptance before closing the loop.
- Can be prone to infeasibility if not correctly designed.
- Requires a robust nonlinear solver.



Limitations of Successive Linearisation (Hill Climbing)



Example – Ethylene Process RTO



Ethylene Process Model

- Detailed feed section and furnace* models.
- Simplified separation section model (shortcut distillation, compressors, flash separation, heaters/coolers, etc.).
- 18 chemical components.

Optimisation Case

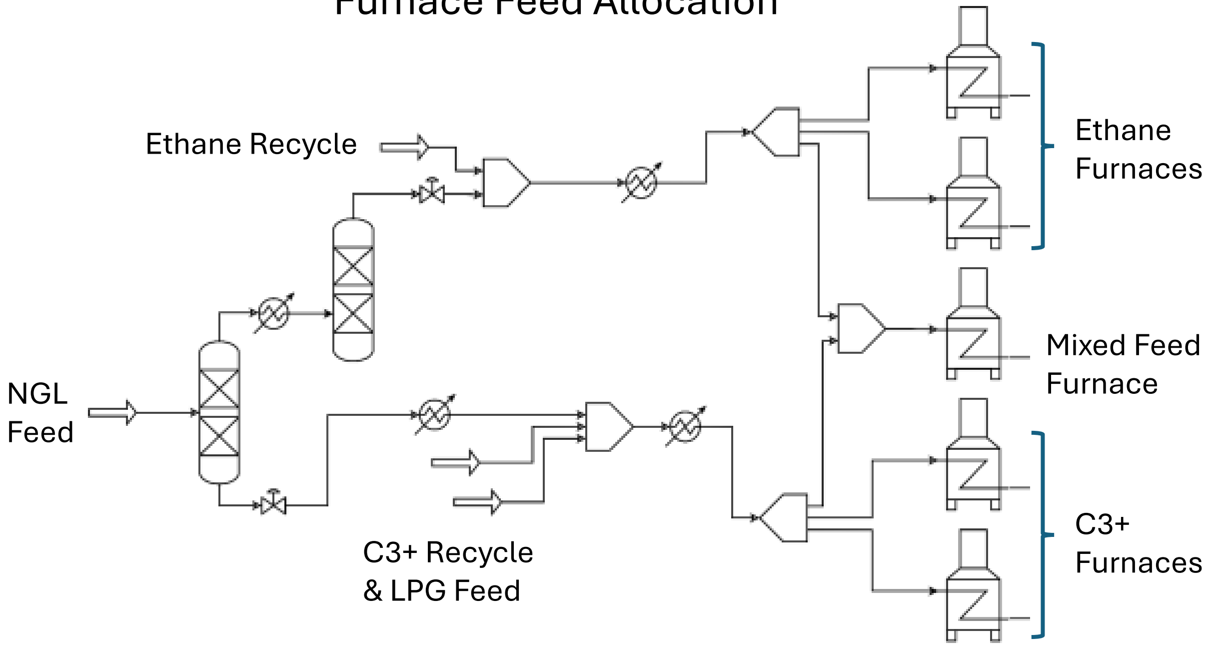
- Determine the optimal feed allocation, furnace conditions, and downstream operation to maximise ethylene production.
- Co-cracking (mixed C2 & C3+) is sub-optimal and should be avoided.

Real-time Optimisation Performance

- 5065 Variables, 2-minute execution cycle.
- Nonlinear, global optimisation.

*In an ethylene process, the cracking reaction takes place in the furnace coils.

Furnace Feed Allocation



Example – Ethylene Process RTO

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Base Case

	f1		f2		f3		f4		f5
Furnace Feed (t/h)	31.11	Furnace Feed (t/h)	31.11	Furnace Feed (t/h)	44.32	Furnace Feed (t/h)	57.52	Furnace Feed (t/h)	57.52
COT (degC)	827.00	COT (degC)	827.00	COT (degC)	850.00	COT (degC)	850.00	COT (degC)	850.00
C2 Conversion (%)	69.63	C2 Conversion (%)	69.63	-		-		-	
-		-		C4 Conversion (%)	76.65	C4 Conversion (%)	74.64	C4 Conversion (%)	74.64
Steam to Hydrocarbon Ratio	0.30	Steam to Hydrocarbon Ratio	0.30	Steam to Hydrocarbon Ratio	0.40	Steam to Hydrocarbon Ratio	0.40	Steam to Hydrocarbon Ratio	0.40

Feed-1		Feed-2		Quench & CGC		Cold Section		Solver	
NGL Feed (t/h)	126.56	Co-crack Percent C2	35.10	CGC Inlet (barg)	0.22	Ethylene Product (t/h)	105.925	Solution Time (seconds)	0
C2 in Feed (mole %)	49.57	Co-crack Percent C3+	64.90	CGC Dischg (barg)	24.41	C2S Btms (t/h)	31.29	Number of Variables	-1
C3 in NGL OHD (mole %)	1.10	Total C3+ Feed (t/h)	143.80	DC3 Reflux Ratio	1.50	Ethane ppm	470	Status Code	4
C2 in NGL Btm (mole %)	1.00	Total C2 Feed (t/h)	77.78	C3 in DC3 Btm (mole %)	0.40	C2= in C2S Btms (mole %)	0.50	Degrees of Freedom	242

Optimised Case

	f1		f2		f3		f4		f5
Furnace Feed (t/h)	43.17	Furnace Feed (t/h)	43.17	Furnace Feed (t/h)	47.77	Furnace Feed (t/h)	48.31	Furnace Feed (t/h)	48.31
COT (degC)	827.24	COT (degC)	827.24	COT (degC)	850.00	COT (degC)	850.00	COT (degC)	850.00
C2 Conversion (%)	66.92	C2 Conversion (%)	66.92	-		-		-	
-		-		C4 Conversion (%)	86.96	C4 Conversion (%)	86.95	C4 Conversion (%)	86.95
Steam to Hydrocarbon Ratio	0.30	Steam to Hydrocarbon Ratio	0.30	Steam to Hyd[illegible]		[illegible] Ratio	0.40	Steam to Hydrocarbon Ratio	0.40

Feed-1		Feed-2		Quench & CGC		Cold Section		Solver	
NGL Feed (t/h)	127.74	Co-crack Percent C2	2.50	CGC Inlet (barg)	0.22	Ethylene Product (t/h)	115.656	Solution Time (seconds)	8.50
C2 in Feed (mole %)	50.67	Co-crack Percent C3+	97.50	CGC Dischg (barg)	24.41	C2S Btms (t/h)	39.41	Number of Variables	5065
C3 in NGL OHD (mole %)	1.07	Total C3+ Feed (t/h)	143.19	DC3 Reflux Ratio	1.50	Ethane ppm	482	Status Code	0
C2 in NGL Btm (mole %)	1.00	Total C2 Feed (t/h)	87.54	C3 in DC3 Btm (mole %)	0.40	C2= in C2S Btms (mole %)	0.50	Degrees of Freedom	14

1. Increased Ethane furnace feed and lower conversion.

2. Ethane to the mixed furnace is reduced to the low limit.

3. Increased Ethylene production.
4. Increased Ethane recycle up to the furnace feed limit for improved yield.

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