Design of Process Operations using Hybrid Dynamic Optimization

Paul I. Barton and Cha Kun Lee

Department of Chemical Engineering
Massachusetts Institute of Technology
77 Massachusetts Avenue
Cambridge, MA 02139

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Outline

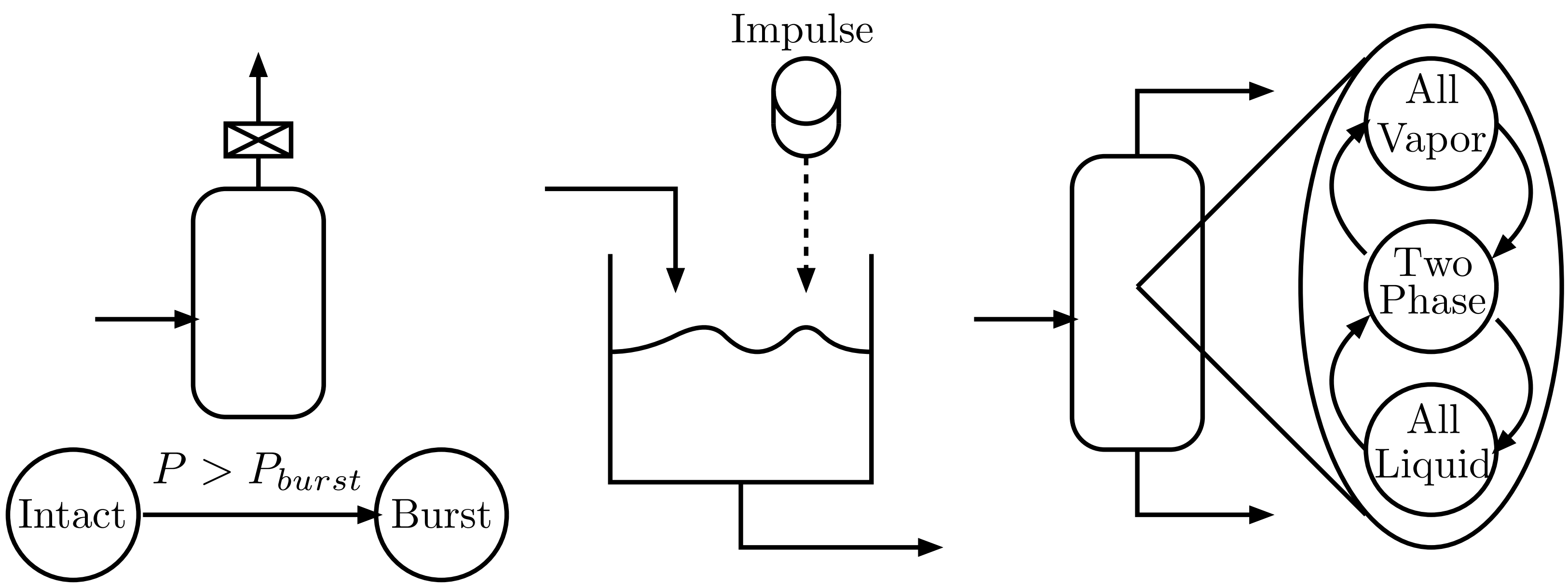
- Modeling, Simulation and Sensitivity Analysis of Process Operations as Hybrid Systems

- Global Dynamic Optimization of Hybrid Systems

- Examples

Hybrid Systems

- Hybrid systems exhibit both ***discrete*** state and ***continuous*** state dynamics



Pressure Vessel with Rupture Disk

Tank with Impulsive Input

Flash Vessel with Phase Transitions

- Accurate dynamic models of process operations, e.g., start-ups and shut-downs are best analyzed using hybrid systems

Modeling Process Operations

- Increasing need for efficient, safe and environmentally friendly process operations

- How will these improvements in process operations be achieved?

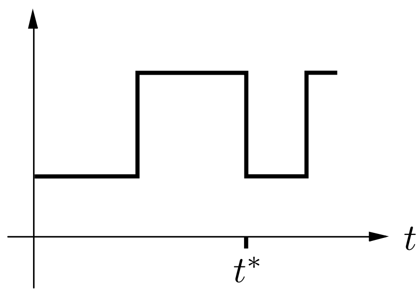
- Detailed physical models, and rigorous analysis and optimization frameworks

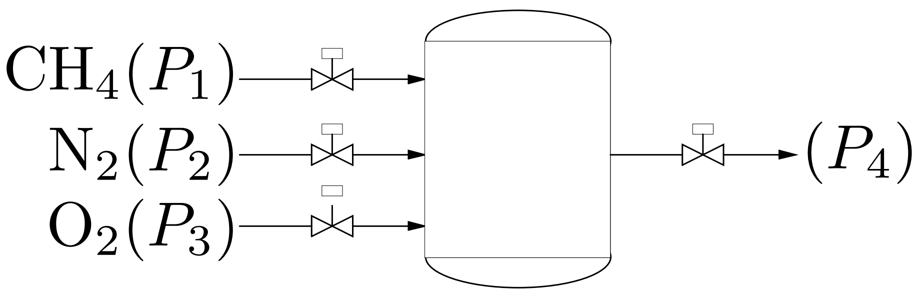
- Continuous process dynamics familiar, but as perturbation from steady-state becomes larger, discrete aspects become more and more important too

- **Hybrid Systems** is the rigorous modeling paradigm for process operations

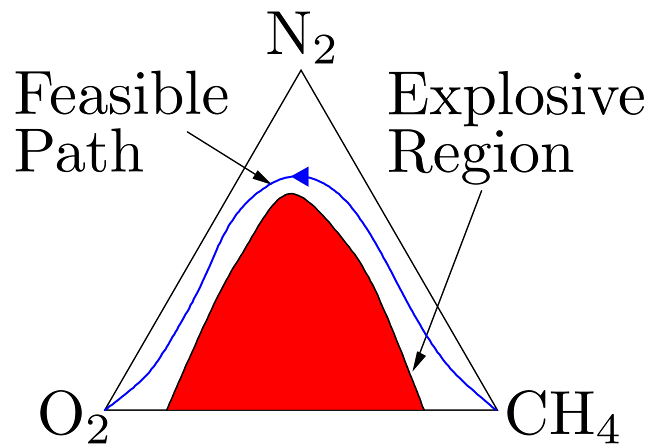
Tank-Changeover Example

$$\min_{u(t),t_f} \; t_f$$





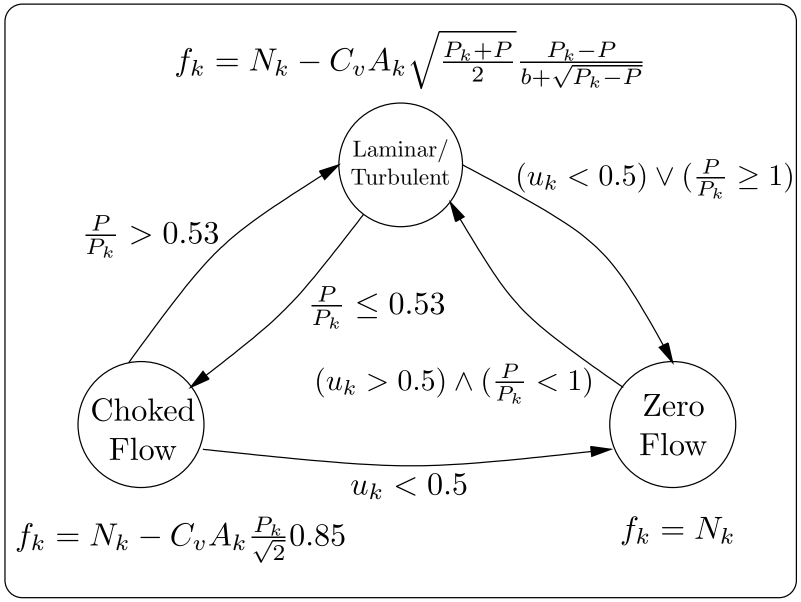
Pressure Vessel



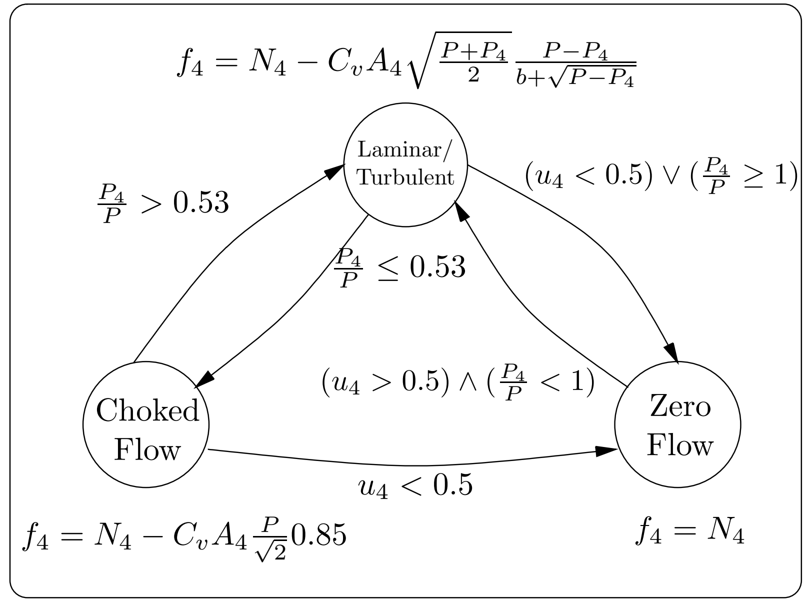
Mole fraction space

- Objective: Minimize the time needed to change from a tank full of methane to one full of oxygen

Tank-Changeover Example



Valve $k \in \{1, 2, 3\}$



Valve 4

For all $i \in I$,

$$f_{(4+i)} = M_i' - N_1 y_{1i} - N_2 y_{2i} - N_3 y_{3i} + N_4 y_{4i}$$

$$f_{(7+i)} = M_i - M_T y_i$$

$$f_{(10+i)} = y_{4i} - y_i$$

$$f_{14} = y_1 + y_2 + y_3 - 1$$

$$f_{15} = PV - M_T RT$$

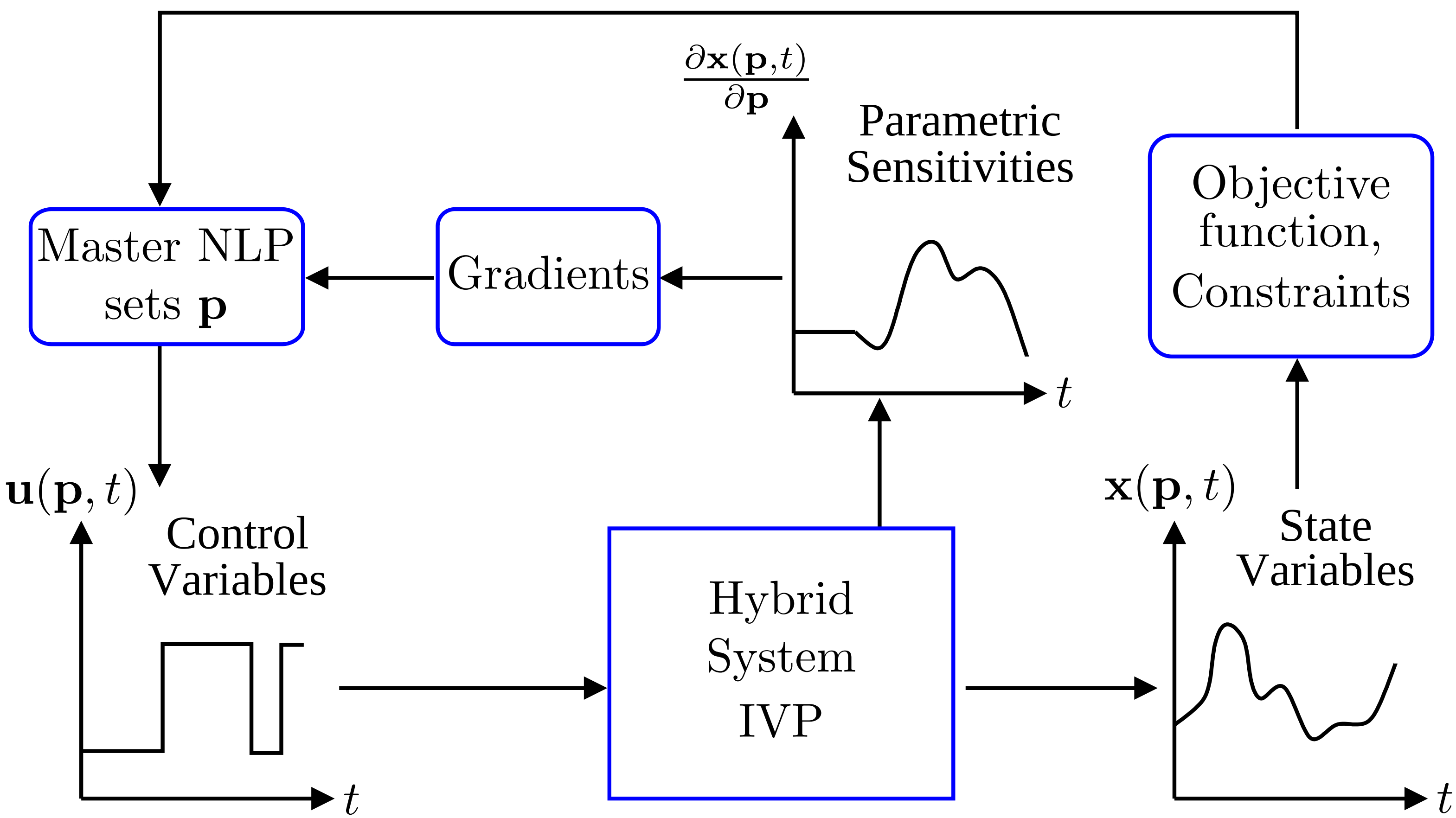
Tank

Tank-Changeover Example

- Controls: on/off signals to valves as a function of time
  - infinite dimensional optimal control problem

- Control parameterization leads to the following:
  - Initial positions of valves known
  - Allow position to switch at finite number of switching times
  - Continuous switching times decision variables in NLP
  - Embeds optimal control if sufficient number of switches allowed

Control parameterization



Parametric Sensitivities of Dynamic Systems

Given a dynamic system expressed in terms of a vector of time invariant parameters p:

$$\dot{x}(p,t) = f(x(p,t), p, t)$$

- then there exists a n_x by n_p matrix of partial derivatives $\frac{\partial x}{\partial p}$ determined by the related matrix differential equations:

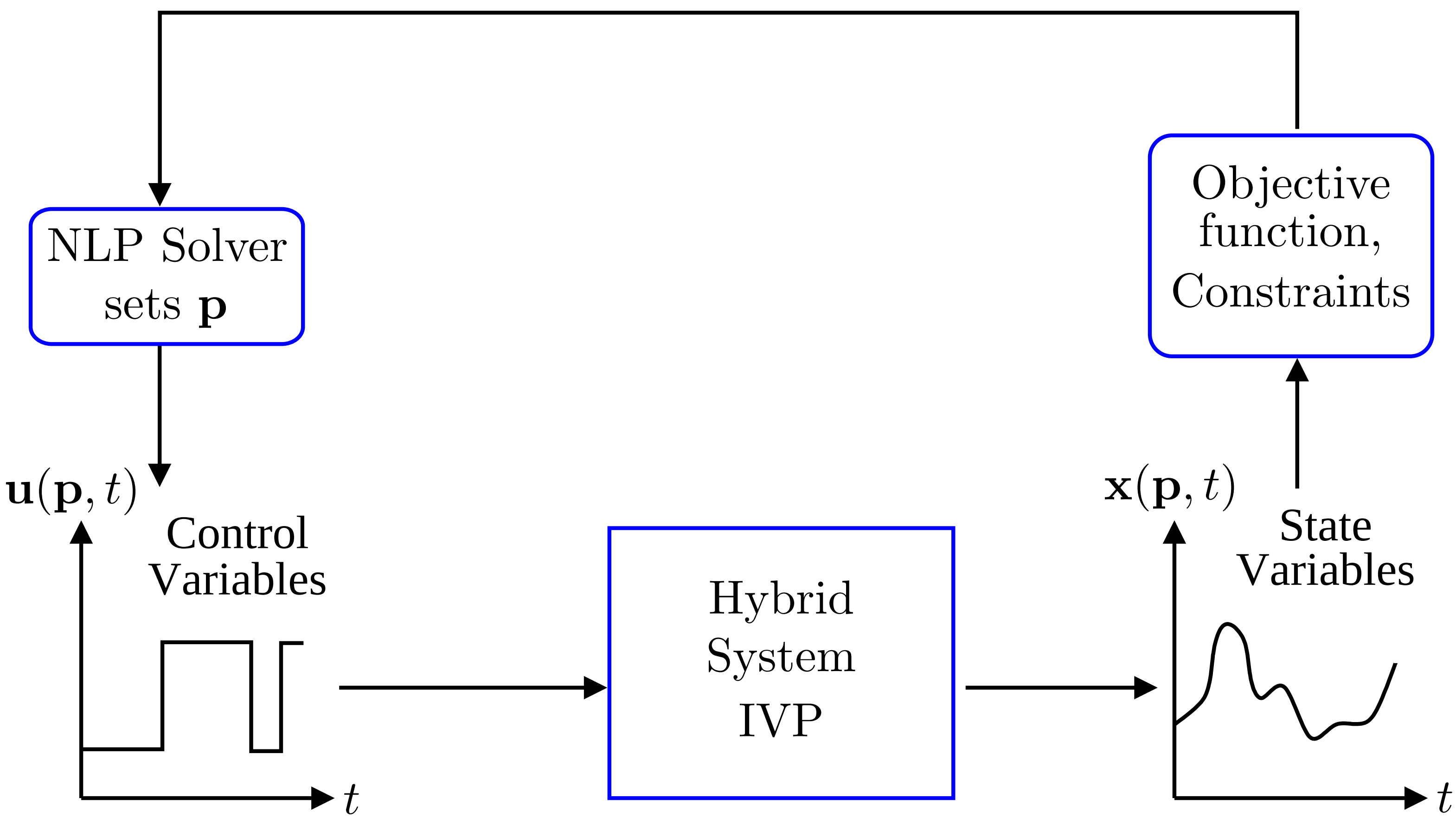
$$\frac{\partial \dot{x}}{\partial p} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial p} + \frac{\partial f}{\partial p}$$

- extension to DAEs straightforward

Parametric Sensitivities of Hybrid Systems

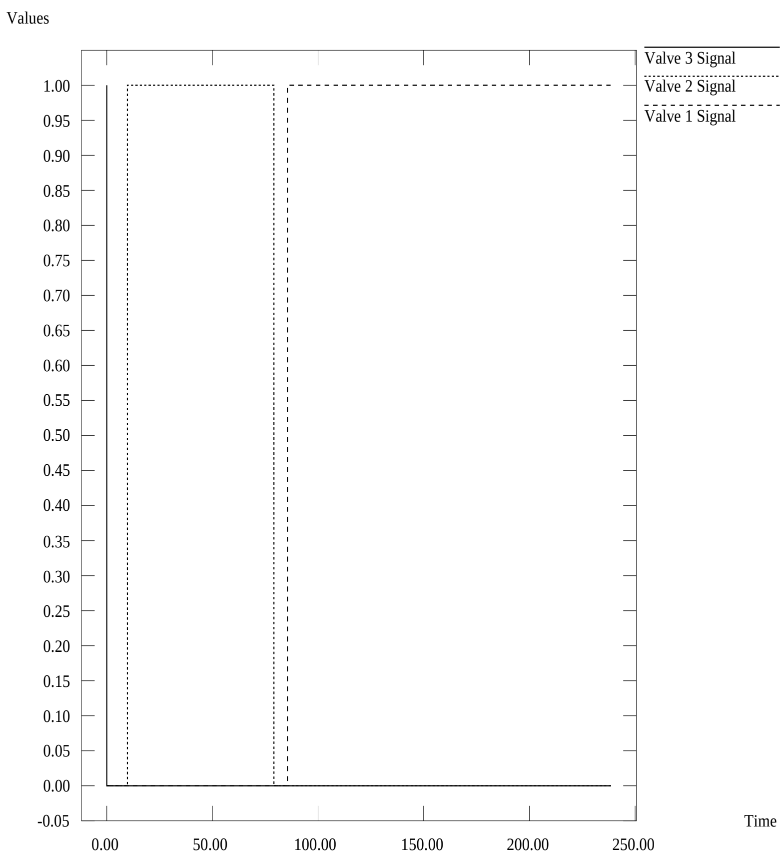
- [Galán et al. (1999)]
- Existence and uniqueness for sensitivities of hybrid systems embedded with:
  - nonlinear ODEs
  - linear time invariant DAEs
- In general, sensitivities of hybrid systems exist *almost everywhere*
- Critical parameter values at which (for example) sequence of events changes qualitatively
  - theorems break down
  - typically associated with discontinuity or nondifferentiability in the objective function

Direct Stochastic Search

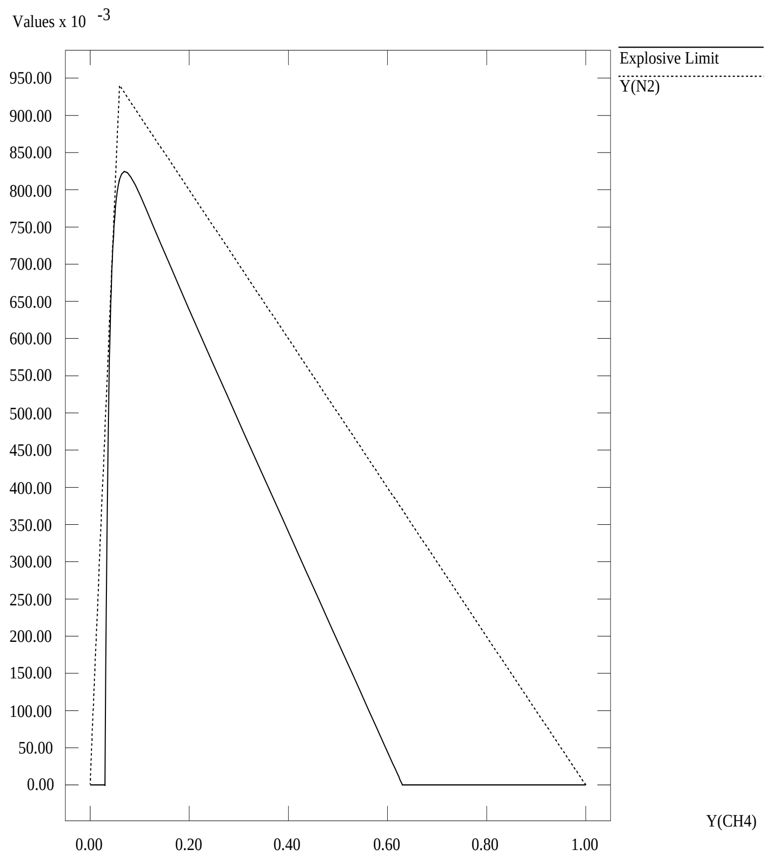


Results from Stochastic Search

Valve Signal Profiles

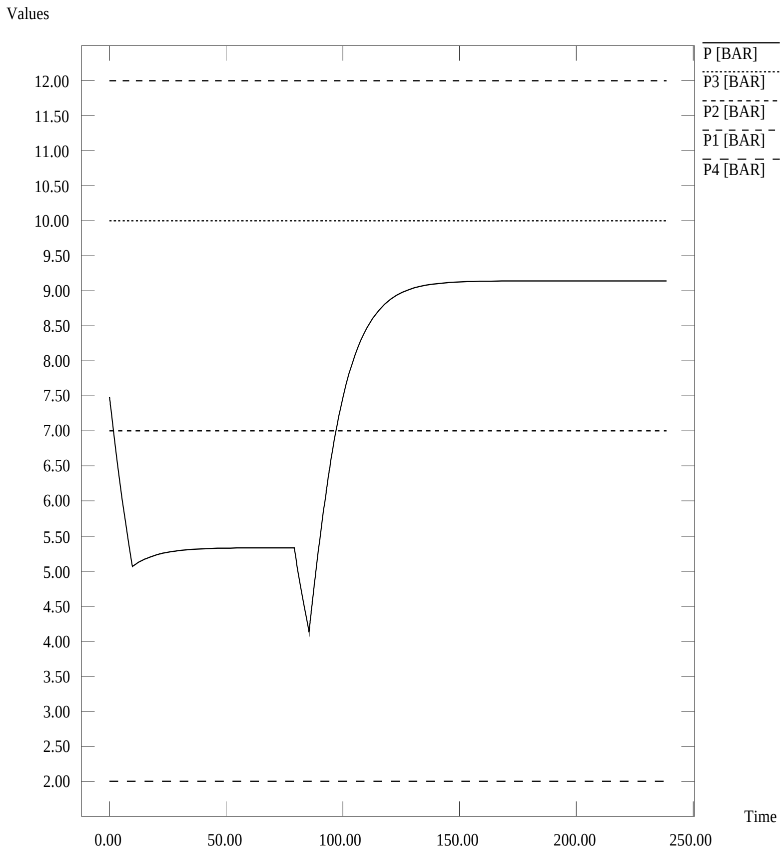


State Space Plot

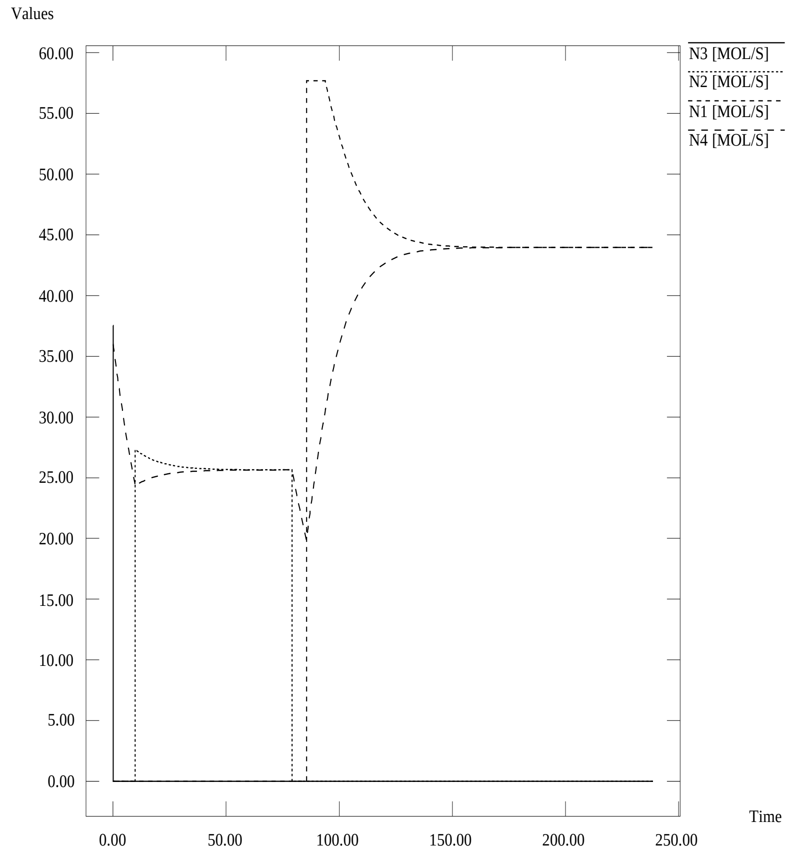


Results from Stochastic search

Pressures



Flow Through Valves

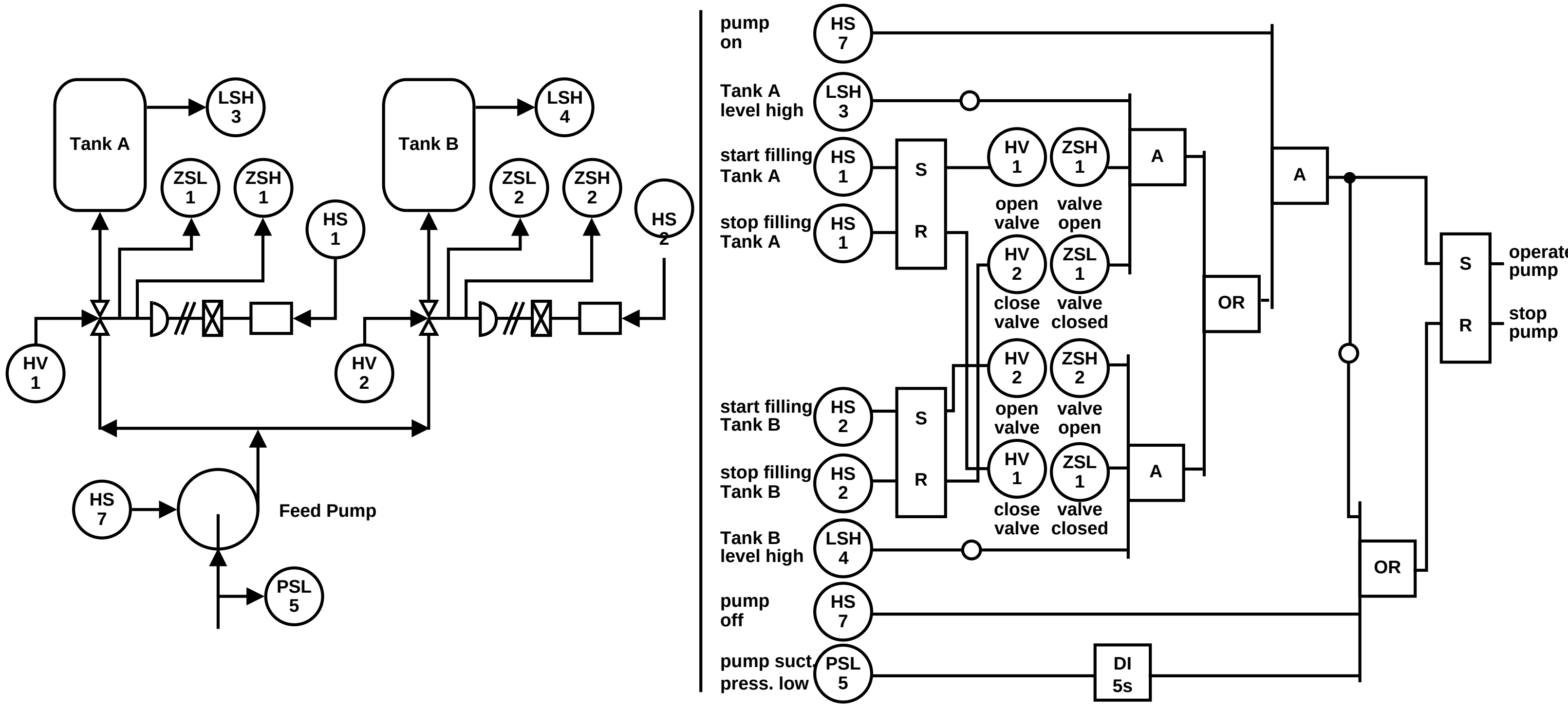


Verification Problems

The direct stochastic search approach

- can deal with nonsmoothness in the master problem
- cannot guarantee the global minimum, can be computationally expensive and can encounter difficulties with constraints

These methods cannot be used for problems where location of the global minimum is crucial, e.g., formal verification of logic based controllers.



Other Approaches

- Discrete time horizon [Bemporad, Borrelli and Morari (2000)]
- Total discretization [Avraam, Shah and Pantelides (1998)]
- Partial discretization
  - Solve directly as an NLP with hybrid system embedded
    - Stochastic methods [Barton, Banga and Galán (2000)]
    - Nonsmooth optimization methods
  - Reformulation of problem as a global Mixed-Integer Dynamic Optimization problem
- Two stage decomposition of switched systems [Xu and Antsaklis (2001)]
- Reachability analysis of hybrid automata [Alur et al. (1995)], [Shakernia, Pappas and Sastry (2000)]

DAEPACK and ABACUSS II

Software packages are available that can robustly handle simulation and sensitivity analysis of hybrid systems:

- ABACUSS II / ABACUSS 3
  - Advanced equation based modeling environment
  - Features include robust sensitivity analysis, sparsity pattern generation, interface to NLP solvers, etc.
- DAEPACK
  - All structural symbolic and numerical information required by modern algorithms for hybrid systems can be generated automatically from a FORTRAN source file
  - Works with very general code: functions, subroutines, common blocks, iterative procedures, etc.
- Very easy to get qualitatively wrong sensitivities using standard codes - must use our symbolic tools

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  - Hybrid systems framework is modeling paradigm for process operations
  - Interesting problems motivate development of global optimization methods

- Global Dynamic Optimization of Hybrid Systems

- Examples

Motivation

Problems that require the global minimum to be located motivate the development of tools for the deterministic global optimization of hybrid systems. A key tool is the ability to

- construct convex relaxations for general, nonlinear Bolza type functions [Singer and Barton (2001)]:

$$F(\mathbf{p}) = \phi\Big(\dot{\mathbf{x}}(\mathbf{p}, t_f), \mathbf{x}(\mathbf{p}, t_f), \mathbf{p}\Big) + \int_{t_0}^{t_f} f\big(\dot{\mathbf{x}}(\mathbf{p}, t), \mathbf{x}(\mathbf{p}, t), \mathbf{p}, t\big)\,\mathrm{d}t$$

  where $\mathbf{x}(\mathbf{p}, t)$ is given by the solution of an embedded dynamic system described by linear time varying ODEs:

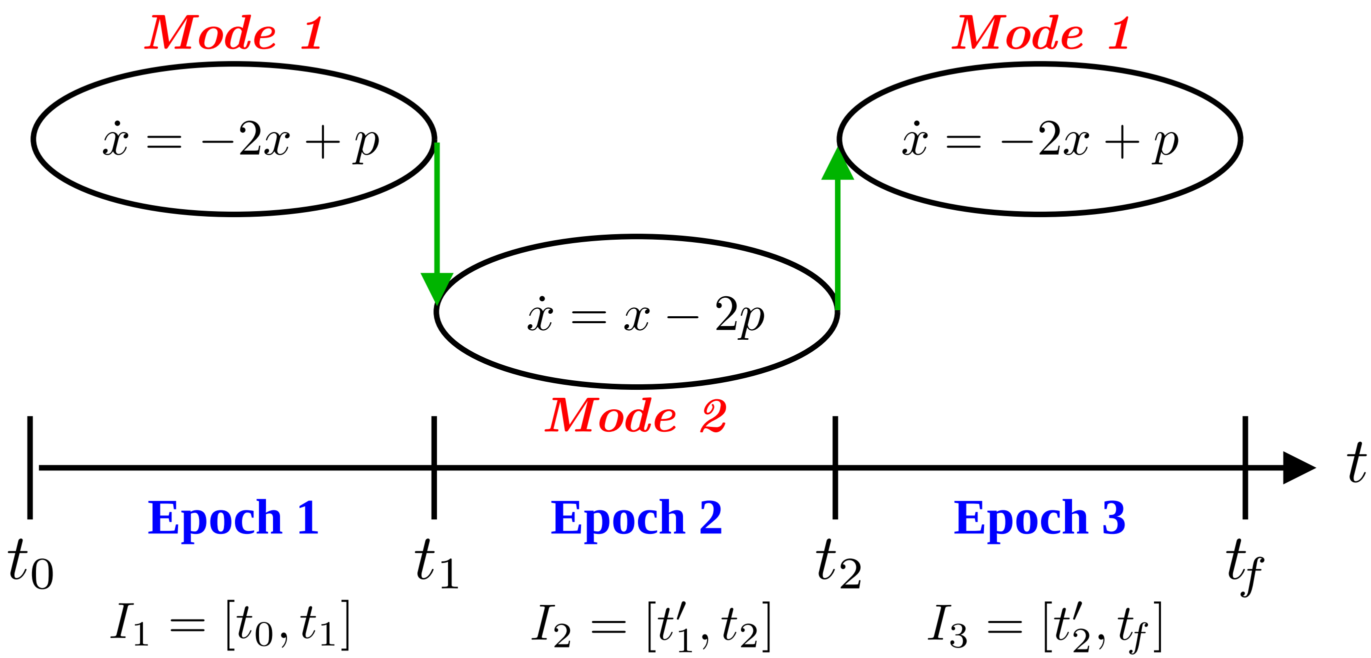
$$\dot{\mathbf{x}}(\mathbf{p}, t) = \mathbf{A}(t)\mathbf{x}(\mathbf{p}, t) + \mathbf{B}(t)\mathbf{p} + \mathbf{q}(t)$$
$$\mathbf{x}(\mathbf{p}, t_0) = \mathbf{E}\mathbf{p} + \mathbf{k}$$

- this has recently been extended to nonlinear ODEs embedded

Hybrid Trajectories

The time horizon is split into contiguous intervals called *epochs*:

- T_μ, the sequence of modes, is called the hybrid mode trajectory
- T_τ, the sequence of epochs, is called the hybrid time trajectory



$$T_\mu = 1, 2, 1 \qquad T_\tau = I_1, I_2, I_3$$

Classes of Hybrid Optimization Problems

- T_μ unchanged and vector field does not jump at events:
  - parametric sensitivities continuous (no jumps)
  - smooth Master NLP

- T_μ unchanged:
  - parametric sensitivities discontinuous functions of time
  - smooth Master NLP

- T_μ to be determined:
  - nonsmooth nonconvex Master NLP
  - decomposition approach - MIDO: Master problem searches over different sequences

Convexity theory for fixed T_μ and T_τ

- With T_μ and T_τ fixed, convexity theory holds and convex relaxations can be constructed.
- Well-known methods for obtaining convex relaxations on Euclidean spaces can be employed, e.g., McCormick's method, αBB. For example:

$$F(p) = \int_0^1 -x^2(p,t)\ \mathrm{d}t$$

$$U(p) = \int_0^1 (x^L(t) + x^U(t))(x^L(t) - x(p,t)) - x^L(t)^2\ \mathrm{d}t$$

- This enables standard global optimization algorithms, such as Branch and Bound, nonconvex Outer Approximation, etc., to be applied.

Example

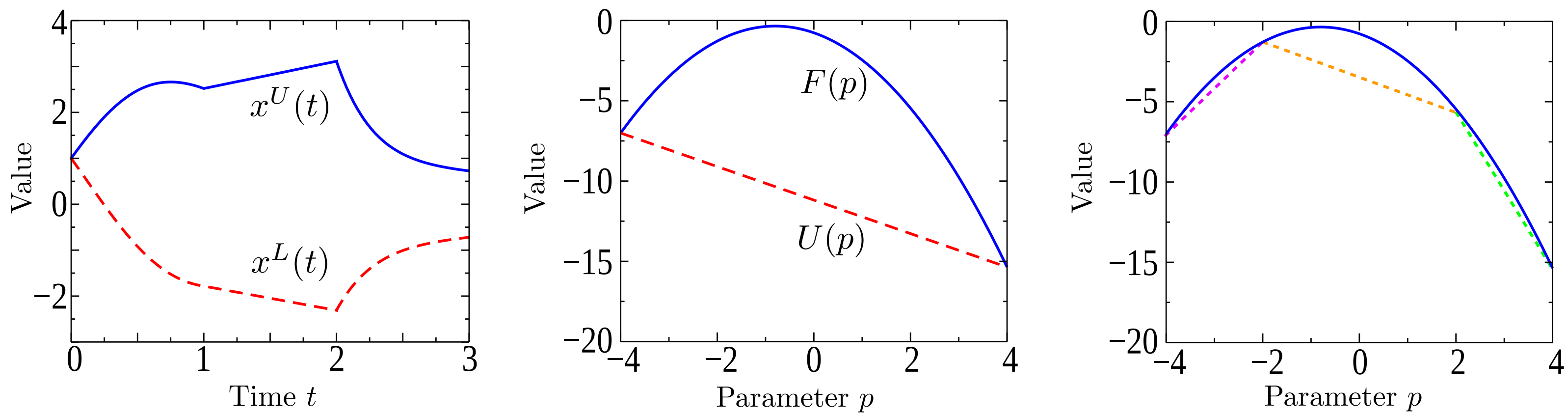
$$\min_{p\in[-4,4]} \quad F(p) = \int_0^3 -x^2(p,t)\ \mathrm{d}t,$$

where $x(p,t)$ is given by the solution to the following hybrid system,

$$\text{Mode 1} \ : \dot{x}(p,t) = -2tx(p,t) + p,$$

$$\text{Mode 2} \ : \dot{x}(p,t) = \frac{x(p,t)+p}{t+10},$$

$x(p,0) = 1$, $T_\mu = \{1,2,1\}$, *and state continuity is enforced at* $t_1 = 1$, $t_2 = 2$.



(a) Implied State Bounds for $p = [-4, 4]$

(b) Objective Function and Convex Underestimator

(c) Branch and Bounding

Varying Sequence of Modes

- Binary decision variables are introduced to represent the sequence of modes:

$$\min_{p,\mathbf{y}} \; F(p,\mathbf{y}) = \int_0^5 -x^2(p,\mathbf{y},t)\ \mathrm{d}t,$$

$$\text{s.t.} \quad y_{11} + y_{21} = 1, \qquad y_{12} + y_{22} = 1, \qquad y_{13} + y_{23} = 1,$$

where $x(p,\mathbf{y},t)$ is given by the solution to the following hybrid system,

$$\text{Mode 1} \;: \dot{x}(p,\mathbf{y},t) = y_{11}(-2tx + p) + y_{21}\left(\frac{x+p}{t+10}\right),$$

$$\text{Mode 2} \;: \dot{x}(p,\mathbf{y},t) = y_{12}(-2tx + p) + y_{23}\left(\frac{x+p}{t+10}\right),$$

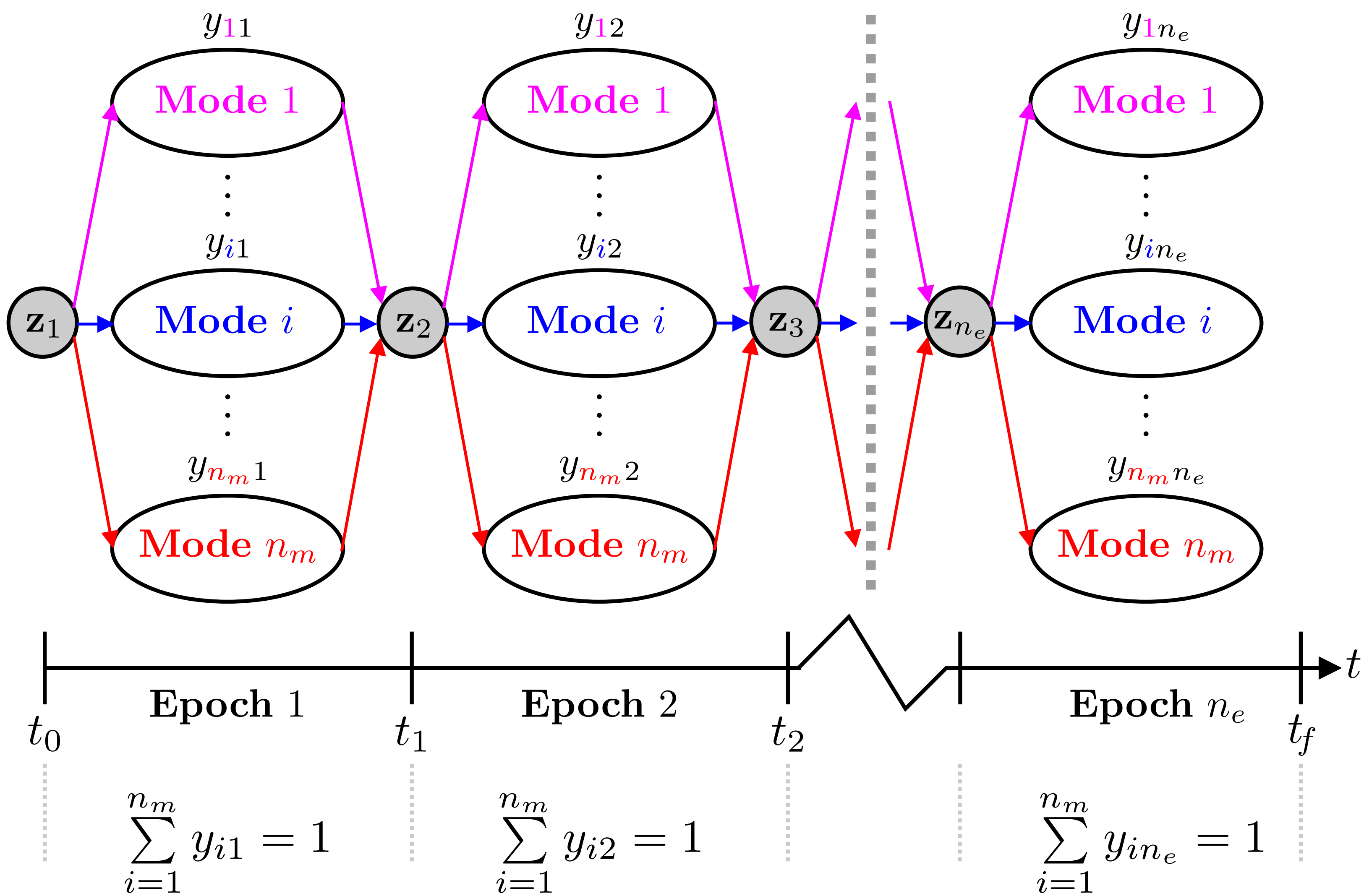
$$\text{Mode 3} \;: \dot{x}(p,\mathbf{y},t) = y_{13}(-2tx + p) + y_{23}\left(\frac{x+p}{t+10}\right),$$

$$x(p,0) = 1,$$

$$p \in P = [-4,4],\ \mathbf{y} \in Y \ \text{binary},$$

$T_\mu = 1,2,3$ *and state continuity is enforced at* $t_1 = 1$ *and* $t_2 = 2.$

Hybrid Superstructure



MIDO Reformulation

- Bilinear terms destroy LTV structure of hybrid system
- Introduce $n_m \times n_e$ dynamic LTV systems:

$$\dot{\mathbf{x}}_{mi}(\mathbf{p}, \mathbf{Z}, t) = \mathbf{A}^{(m)}(t)\mathbf{x}_{mi}(\mathbf{p}, \mathbf{Z}, t) + \mathbf{B}^{(m)}(t)\mathbf{p} + \mathbf{q}^{(m)}(t),$$
$$\forall\ m \in M,\ i = 1, \ldots, n_e,$$

  M is the set of n_m modes, and n_e is the total number of epochs

- Introduce $n_x \times n_e$ additional parameters to represent initial conditions for each epoch:

$$\mathbf{z}_1 = \mathbf{E}_0\mathbf{p} + \mathbf{k}_0,$$
$$\mathbf{z}_i = \mathbf{x}_{mi}(\mathbf{p}, \mathbf{Z}, t_i'), \quad \forall\ m \in M,\ i = 1, \ldots, n_e.$$

- Bilinearities shifted to constraints:

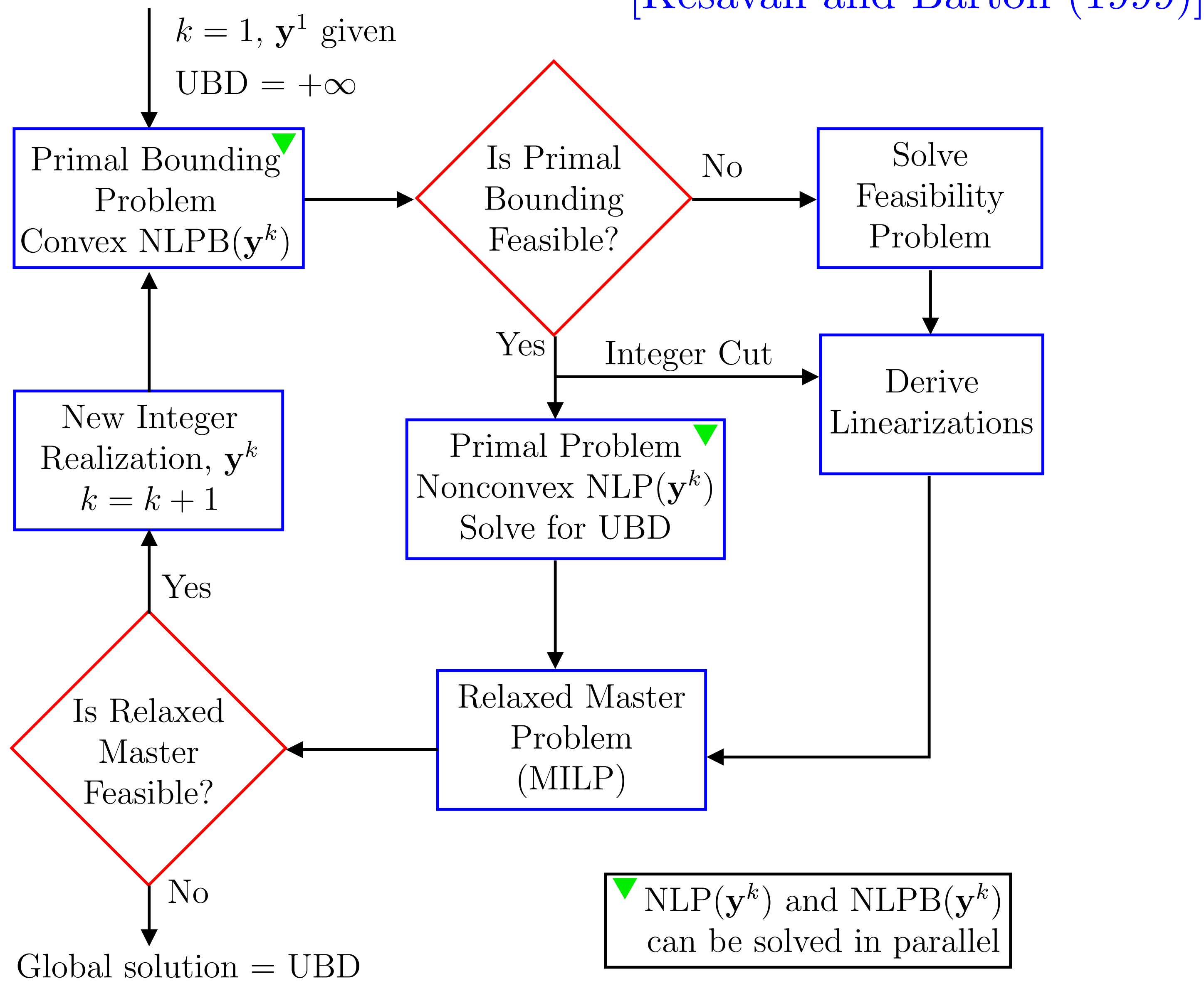
$$\mathbf{z}_{i+1} = \mathbf{D}_i \left(\sum_{m=1}^{n_m} y_{mi}\mathbf{x}_{mi}(\mathbf{p}, \mathbf{Z}, t_i) \right) + \mathbf{E}_i\mathbf{p} + \mathbf{k}_i,\ \forall\ i = 1, \ldots, n_e - 1.$$

MIDO Reformulation

- Reformulated problem is a MIDO with a set of LTV ODE systems
- Using nonconvex OA, MIDO is solved as a nonconvex MINLP
- Ability to construct convex lower bounding MINLP is key, resulting in the following subproblems in OA:
  - Primal: noncovex NLP, provides upper bound
  - Primal Bounding: convex NLP, potentially reduces number of primal problems to solve
  - Relaxed Master: MILP, provides lower bound

Nonconvex Outer Approximation

[Kesavan and Barton (1999)]



Solving the MIDO

- Exact linearizations can be obtained for bilinear/trilinear constraints introduced in the reformulation

- Additional linearizations in the relaxed Master problem only have to be constructed for nonlinear terms in the objective function and constraints

- Mode assignment constraints constitute S0S1 sets and can be exploited when solving the relaxed Master problem

- It suffices to add only linearizations of the active constraints in the primal bounding problem to the relaxed Master problem - not all $n_m \times n_e$ sets of dynamic systems have to be solved

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  - Interesting problems motivate development of global optimization methods
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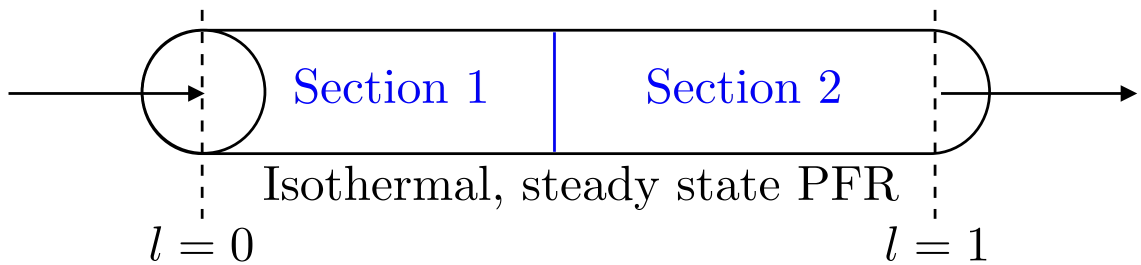
Catalyst Loading Problem

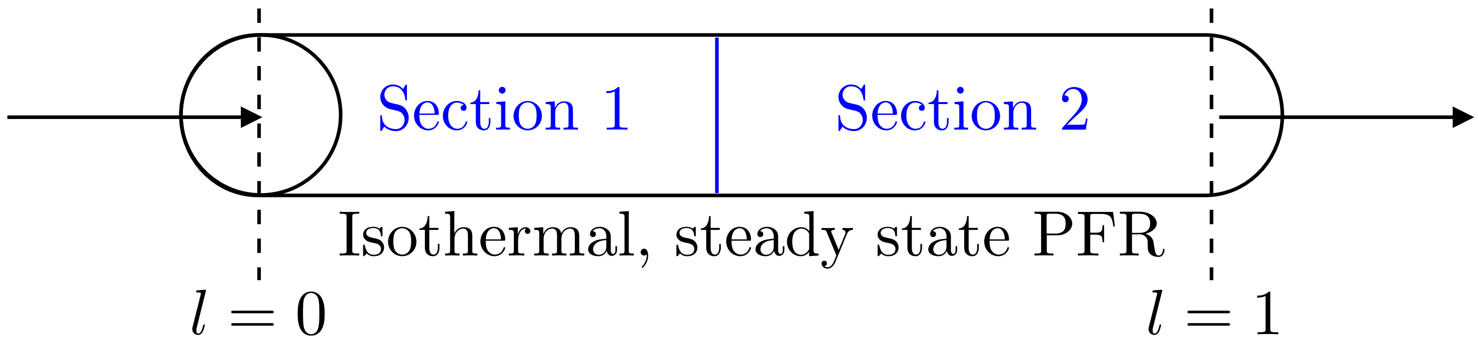
- Given
  - an isothermal PFR at steady state,
  - 2 loading bays,
  - 3 possible kinds of catalyst on support,



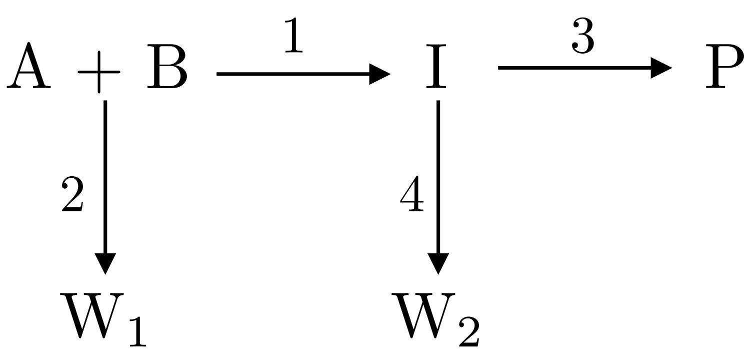
  determine the optimal catalyst loading profile for the PFR that will maximize the profit.

- This can be viewed as an optimization problem with a hybrid system embedded.
- Optimal T_μ corresponds to the optimal choice of catalyst loading.

Catalyst Loading Problem



Reaction scheme

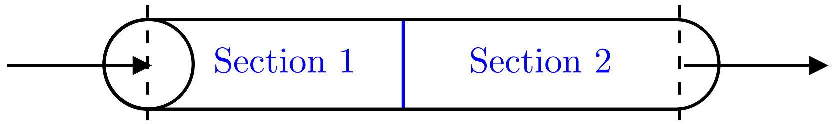


Kinetics

$$
\begin{aligned}
\dot{x}_{\mathrm{A}} &= -(k_1 + k_2)x_{\mathrm{A}} \\
\dot{x}_{\mathrm{B}} &= -(k_1 + k_2)x_{\mathrm{B}} \\
\dot{x}_{\mathrm{W}_1} &= k_2 x_{\mathrm{A}} \\
\dot{x}_{\mathrm{I}} &= k_1 x_{\mathrm{A}} - (k_3 + k_4)x_{\mathrm{I}} \\
\dot{x}_{\mathrm{W}_2} &= k_4 x_{\mathrm{I}} \\
\dot{x}_{\mathrm{P}} &= k_3 x_{\mathrm{I}}
\end{aligned}
$$

Catalyst Loading Problem

$x_{\mathrm{A}}(0) = 1000$ $\qquad$ $x_{\mathrm{P}}(1) - 0.01x_{\mathrm{W}_1}(1) - 0.1x_{\mathrm{W}_2}(1)$



Catalyst

	k_1	k_2	k_3	k_4
1	2.098	1.317	0.021	0.033
2	29.53	110.2	0.295	0.079
3	182.6	2325	1.826	0.143

	k_1/k_2	k_3/k_4
1	1.594	0.627
2	0.268	3.728
3	0.079	12.729

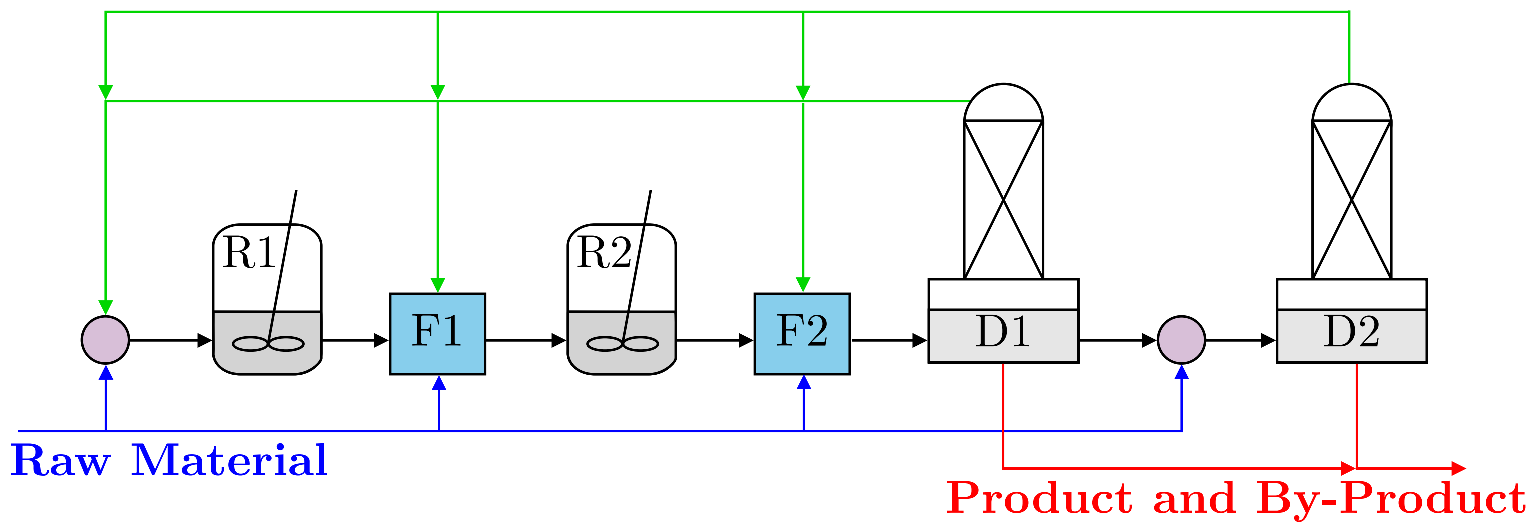
$$\max_{T_\mu} \quad x_{\mathrm{P}}(1) - 0.01x_{\mathrm{W}_1}(1) - 0.1x_{\mathrm{W}_2}(1)$$

$\longrightarrow$ $T_\mu = 1, 3$ $\qquad$ $F = 290.4$

- For 10 catalyst sections, we get $T_\mu = 1, 1, 1, 1, 3, 3, 3, 3, 3, 3$ with $F = 296.5$

Batch Reaction and Distillation

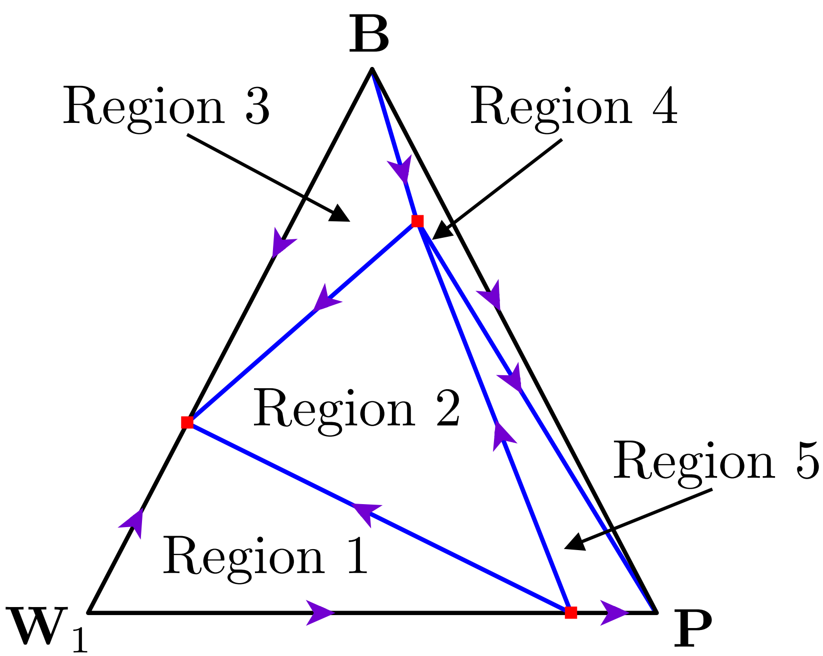
- Building on the previous example, we consider a batch reaction and distillation problem:



- The objective is to minimize raw material and waste treatment costs while maintaining a desired level of production of product.
- Amount of raw material, recycle flows, and choice of catalyst are optimization variables. Each reactor's run is for 1.5h.

Batch Reaction and Distillation

- Components B, W_1 and P form a ternary and 2 binary azeotropes:



	Azeotrope Composition		
	W_1-P	B-W_1-P	B-W_1
B		0.72	0.35
W_1	0.15	0.06	0.65
P	0.85	0.22	

Product Cut Sequence

1 : { A, W_1-P, W_1, I, B-W_1, W_2 }

2 : { A, W_1-P, B-W_1-P, I, B-W_1, W_2 }

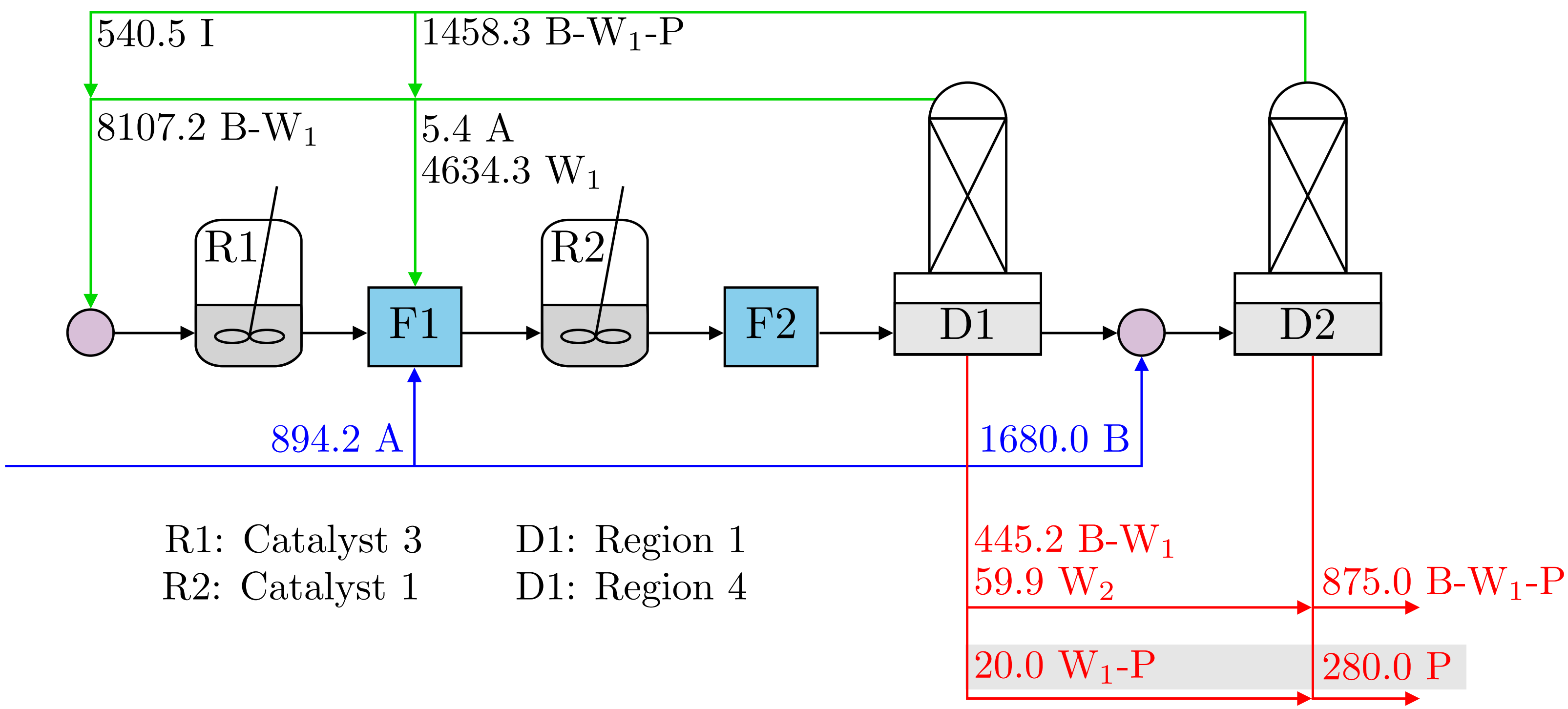
3 : { B, A, B-W_1-P, I, B-W_1, W_2 }

4 : { B, A, B-W_1-P, I, P, W_2 }

5 : { A, W_1-P, B-W_1-P, I, P, W_2 }

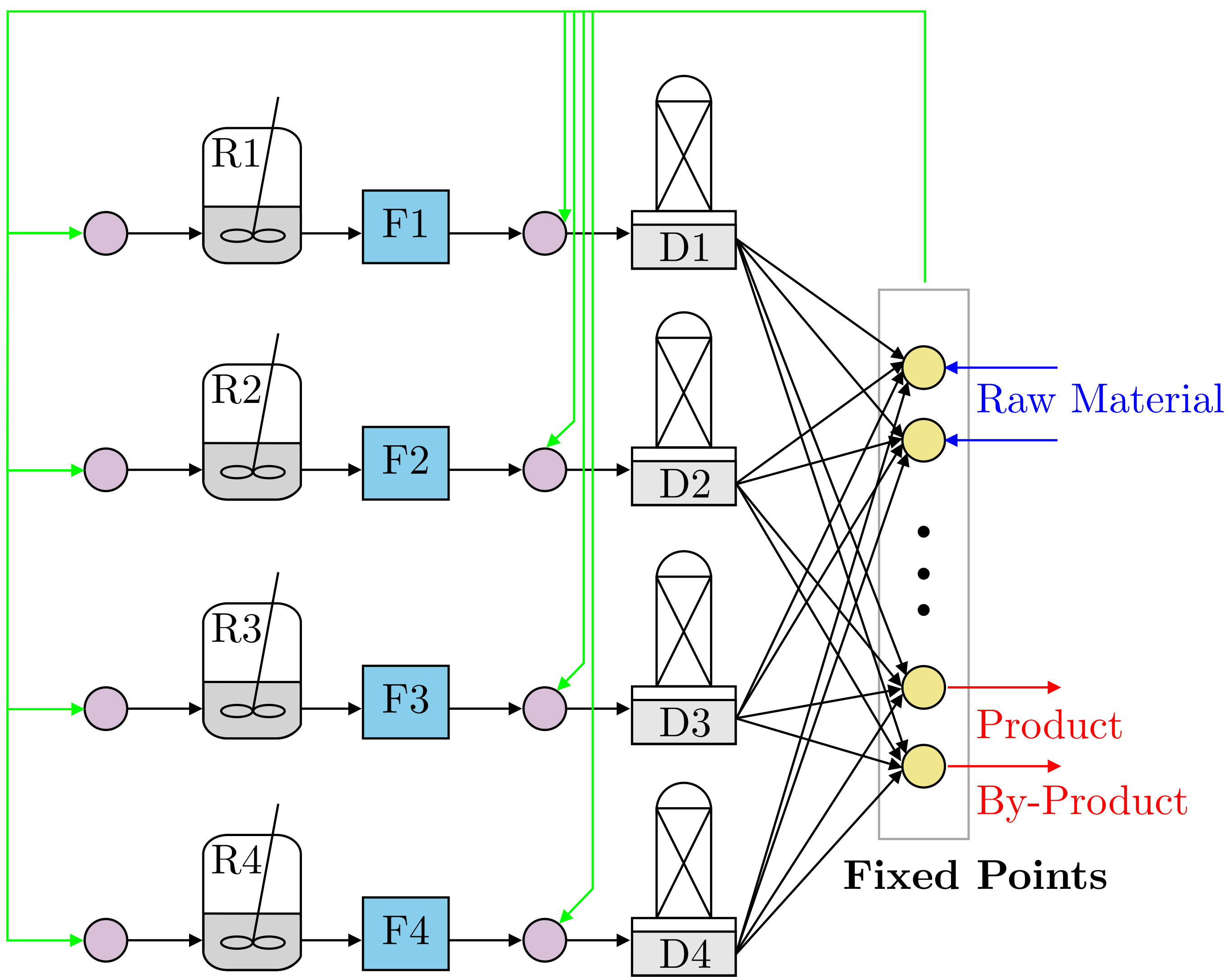
Batch Reaction and Distillation

- Process constraints:
  - molar solvent to reactant ratio (B, W_1, W_2 : A, I) $\geq$ 15
  - at least 2 times B in excess of A
  - 99% pure P
- Optimal solution: (Cost of \$5.061M to produce 300 kmol P)



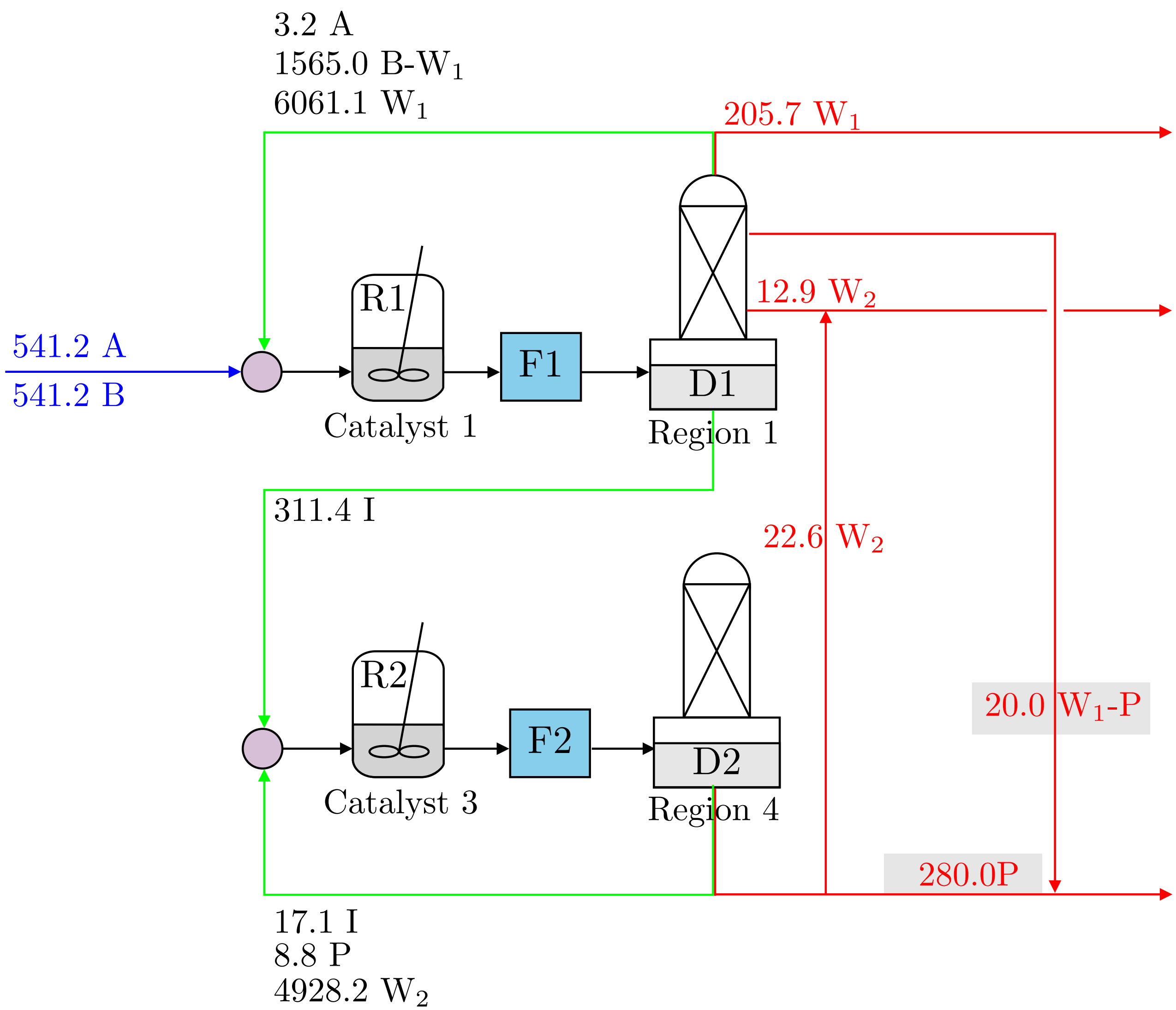
Batch Reaction and Distillation

- Postulating a superstructure with 4 trains:



Batch Reaction and Distillation

- Optimal solution: (Cost of $1.905M to produce 300 kmol P)



Conclusion

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  - Catalyst loading problem
  - Batch reaction and distillation problem

Future Work

- Varying T_τ

- Development of convexity theory for nonlinear dynamic systems (done)

- Extension of results for nonlinear hybrid systems

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