Nonsmooth Differential-Algebraic Equations

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Dynamic Modeling Frameworks in PSE

- Trade-off: applicability vs. ease of modeling & solving

Smooth Models

Limited applicability

Easy to model and solve

Derivative information

Strong existence & uniqueness theory

Nonsmooth Models

Broad applicability

Easy to model and solve

Generalized derivative information

(recently) Strong existence & uniqueness theory

Hybrid (Discrete/ Continuous) Models

(near) Universal applicability

Often challenging to model and solve

Limited derivative information

Pathological behaviors (hard to exclude a priori)

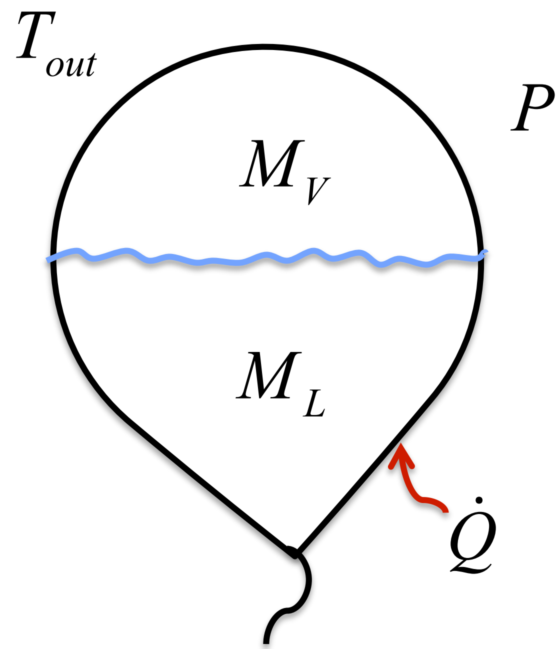
Smooth approximation models

Complementarity systems

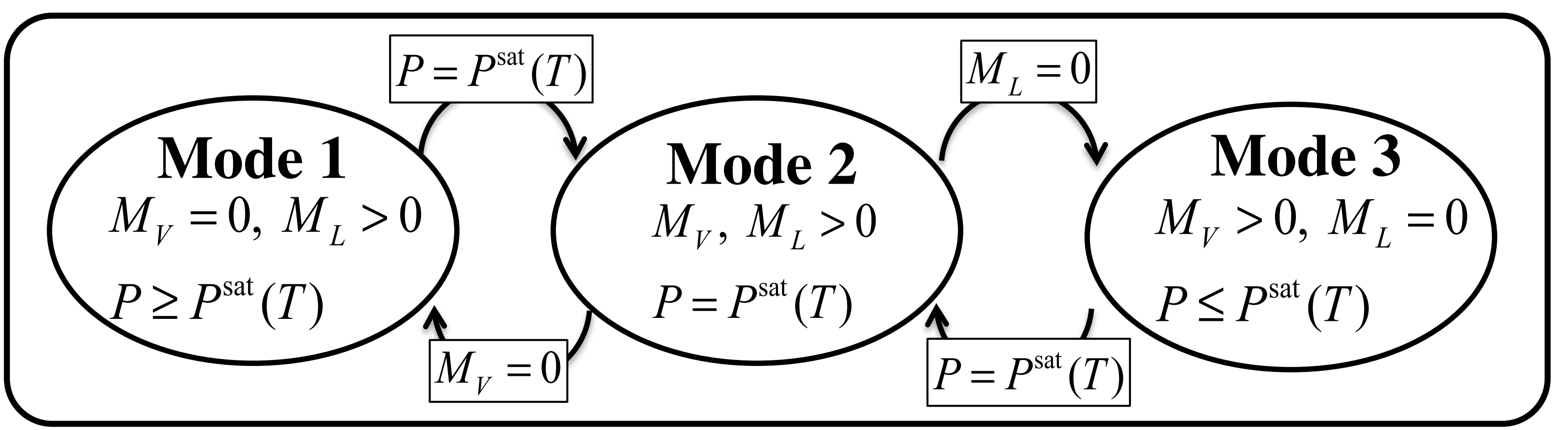
Hybrid Automaton Framework

- Simple const. *P* flash process:

$$\dot{H}(t) = U\left(T_{out} - T(t)\right)$$
$$M = M_L(t) + M_V(t)$$
$$H(t) = Mh_V(t) - M_L(t)\Delta h_{vap}\left(T(t)\right)$$
$$h_V(t) = Cp\left(T(t) - T_0\right)$$
$$\log\left(P^{sat}(t)\right) = A - B/\left(T(t) + C\right)$$
$$\vdots$$

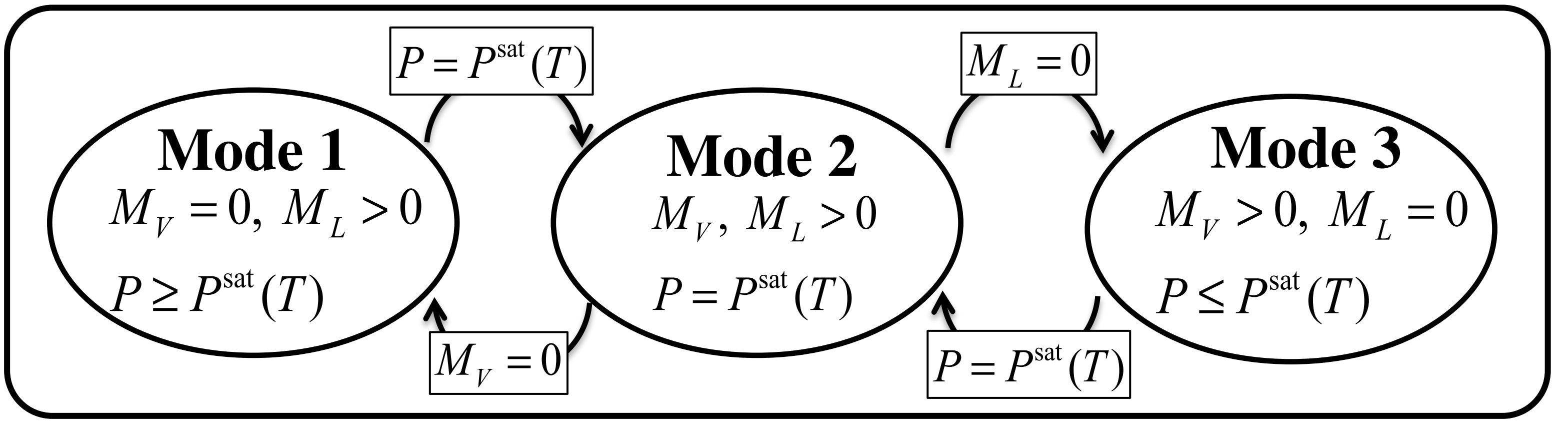


   - DAE embedded in hybrid automaton



Hybrid vs. Nonsmooth

- Hybrid automaton formulation



- "Continuous" disjunction:

$$\begin{bmatrix} M_V(t) = 0 \\ M_L(t) > 0 \\ P \geq P^{\text{sat}}(T(t)) \end{bmatrix} \otimes \begin{bmatrix} M_V(t) > 0 \\ M_L(t) > 0 \\ P = P^{\text{sat}}(T(t)) \end{bmatrix} \otimes \begin{bmatrix} M_V(t) > 0 \\ M_L(t) = 0 \\ P \leq P^{\text{sat}}(T(t)) \end{bmatrix}$$

Hybrid vs. Nonsmooth

- "Continuous" disjunction:

$$\begin{bmatrix} M_V(t)=0 \\ M_L(t)>0 \\ P \geq P^{\text{sat}}(T(t)) \end{bmatrix} \otimes \begin{bmatrix} M_V(t)>0 \\ M_L(t)>0 \\ P = P^{\text{sat}}(T(t)) \end{bmatrix} \otimes \begin{bmatrix} M_V(t)>0 \\ M_L(t)=0 \\ P \leq P^{\text{sat}}(T(t)) \end{bmatrix}$$

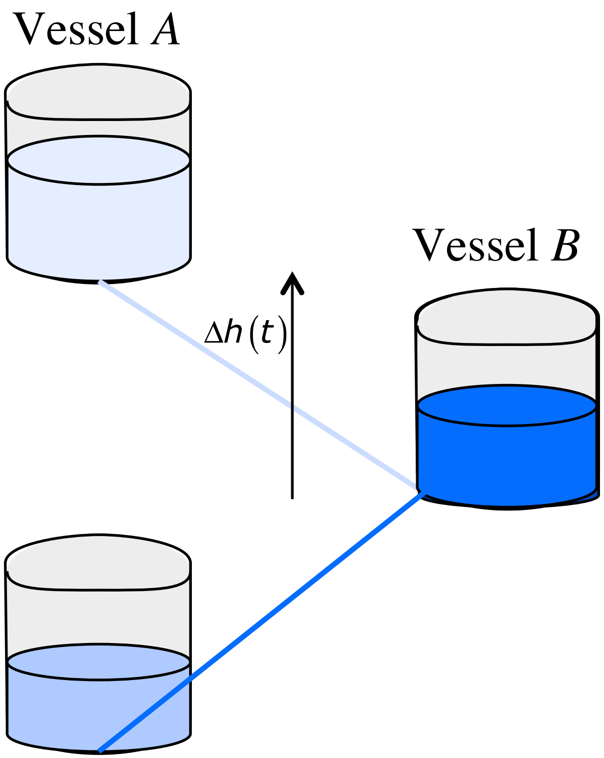
- Nonsmooth equation:

$$0=\operatorname{mid}\left(M_V(t), P-P^{\text{sat}}(T(t)), -M_L(t)\right)$$

Nonsmooth Models: Applications

- Intensive properties with flow reversals
- Flow transitions (laminar, turbulent, choked)
- Thermodynamic phase changes
- Crystallization kinetics: growth vs. dissolution
- Flow control devices, diodes
- Irregularities in vessel geometry
- Dynamic flux balance analysis (DFBA) systems
  - e.g., aerobic to anaerobic switch
- Various "elements" of controllers
- Protecting domains of functions (abs)
- Piecewise properties
- etc., etc.

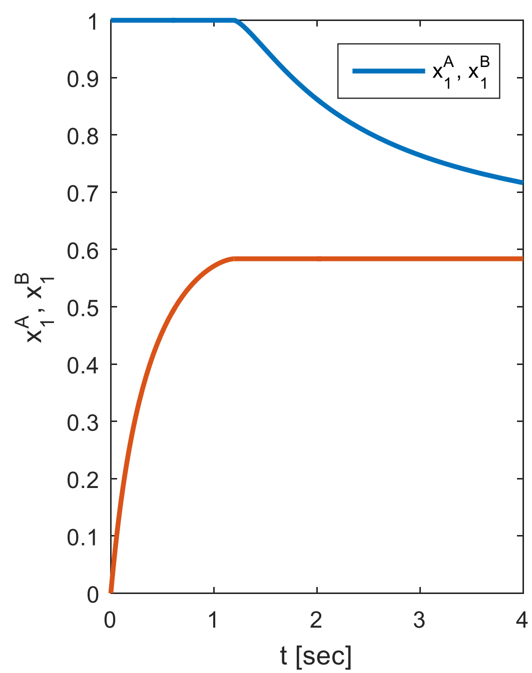
Flow Reversal: Intensive Properties

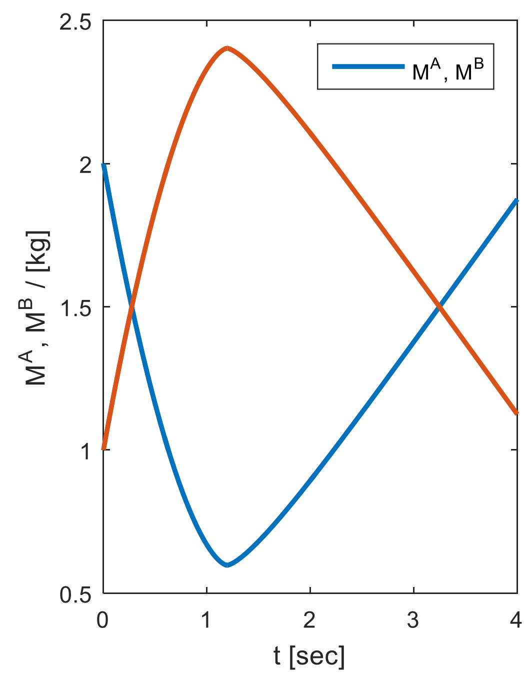


$$\frac{dM_i^A}{dt}(t) = -\left(\max\left(F_{out}^A(t),0\right)x_i^A + \min\left(F_{in}^B(t),0\right)x_i^B\right)$$

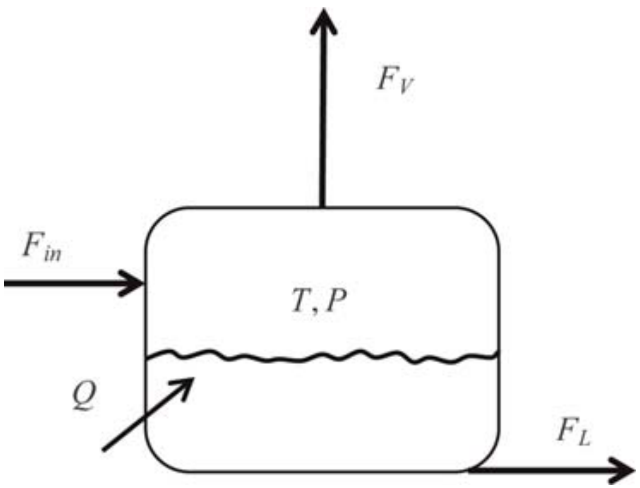
$$\frac{dM_i^B}{dt}(t) = -\frac{dM_i^A}{dt}(t); \qquad F_{out}^A(t) = F_{in}^B(t)$$

$$F_{out}^A(t) = c\frac{h^A(t) - h^B(t) + \Delta h(t)}{\sqrt{\left|h^A(t) - h^A(t) + \Delta h(t)\right| + \varepsilon}}$$





Multi-component Dynamic VLE



Thermodynamic phase equilibrium:

$$y_i(t) = k_i(t)x_i(t)$$

$$0 = \text{mid}\left(\frac{M_V(t)}{M_V(t)+M_L(t)}, \sum_{i=1}^{n_C} x_i(t) - \sum_{i=1}^{n_C} y_i(t), \frac{M_V(t)}{M_V(t)+M_L(t)} - 1\right)$$

Mass and energy balances:

$$\frac{dM_i}{dt}(t) = F_{in}(t)z_i(t) - F_L(t)x_i(t) - F_V(t)y_i(t)$$

$$\frac{dU}{dt}(t) = F_{in}(t)h_{in}(t) - F_L(t)h_L(t) - F_V(t)h_V(t) + Q(t)$$

$$M_i(t) = M_L(t)x_i(t) + M_V(t)y_i(t)$$

$$\sum_{i=1}^{n_C} M_i(t) = M_L(t) + M_V(t)$$

$$H(t) = M_L(t)h_L(t) + M_V(t)h_V(t)$$

$$H(t) = U(t) + P(t)V$$

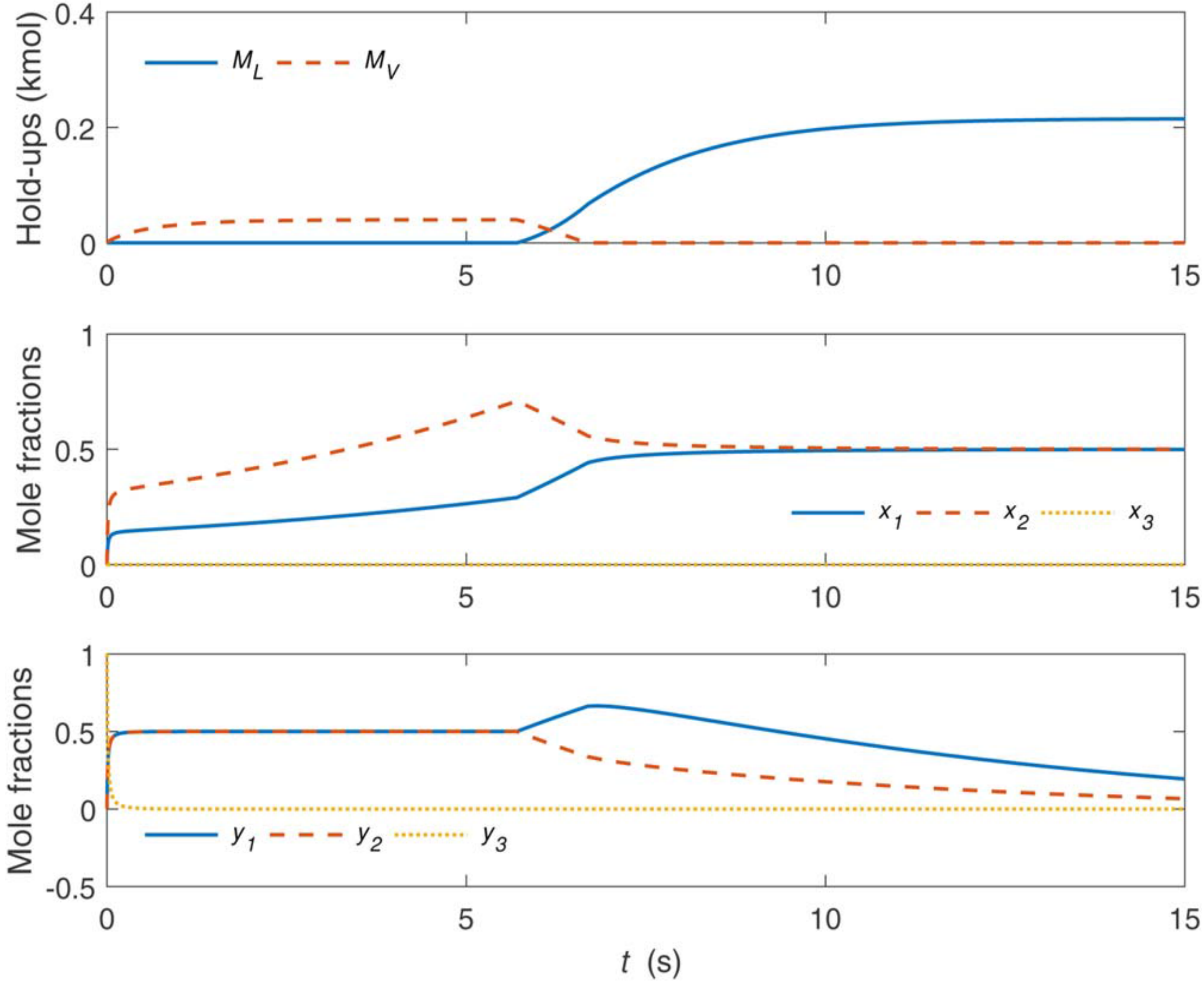
Flow control:

$$F_V(t) = c_v \min\left(V_V^{\min}, V_V(t)\right)\max\left(0, \frac{P(t)-P_0}{\sqrt{\left|P(t)-P_0\right| + \varepsilon}}\right)$$

$$F_L(t) = c_l \min\left(V_L^{\min}, V_L(t)\right)\max\left(0, \frac{K_L(t)}{\sqrt{\left|K_L(t)\right| + \varepsilon}}\right)$$

$$K_L(t) = g\frac{V_L(t)}{A} + \frac{P(t)-P_0}{\rho_L(t)}$$

Multi-component Phase Change



$$M_L = 0$$

$$\sum_{i=1}^{n_C} x_i(t) \leq 1$$

$$M_V = 0$$

$$\sum_{i=1}^{n_C} y_i(t) \leq 1$$

Sahlodin, Watson, Barton, *AIChE J. 62 (2016): 3334-3351*

Crystallization Kinetics

- With the development of continuous crystallization processes, dissolution has to be considered in dynamic models of crystal size distribution:

$$\frac{\partial(Vn)}{\partial t}(t,z)+K(t)\frac{\partial(Vn)}{\partial z}(t,z)=Q_{in}(t)n_{in}(t,z)-Q_{out}(t)n(t,z)$$

$$S(t)=\left(\mathrm{x}_{\mathrm{i}}(t)-x_i^{sat}\right)/\,x_i^{sat},\quad \boxed{K(t)=\min\left(k_D S(t)\left|S(t)\right|^{n_D-1},k_G\left|S(t)\right|^{n_G}\right)}$$

- With finite volume discretization of the size coordinate:

$$\frac{dN_j}{dt}(t)+\frac{1}{\Delta z}\Big(G(t)\big(N_j(t)-N_{j-1}(t)\big)+D(t)\big(N_{j+1}(t)-N_j(t)\big)\Big)=Q_{in}(t)n_{j,in}(t)-Q_{out}(t)n_j(t),\qquad j=2,\ldots,m-1$$

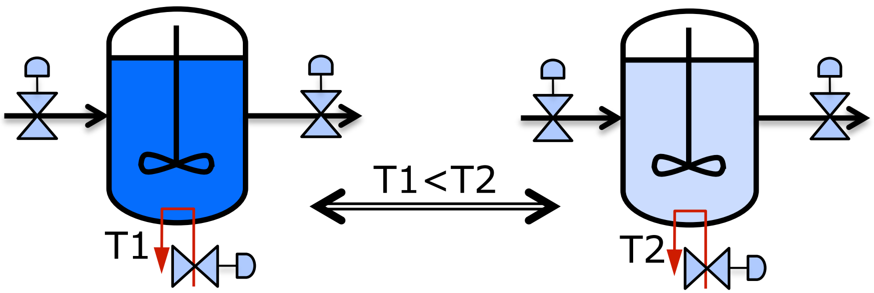
$$\boxed{\begin{aligned}G(t)&=\max\left(0,k_G S(t)\left|S(t)\right|^{n_G-1}\right)\\ D(t)&=\min\left(k_D S(t)\left|S(t)\right|^{n_D-1},0\right)\end{aligned}}$$

$N_j \equiv Vn_j$,

n_j – density of crystals of size $(j-1)\Delta L < L < j\Delta L$

Crystallization Kinetics

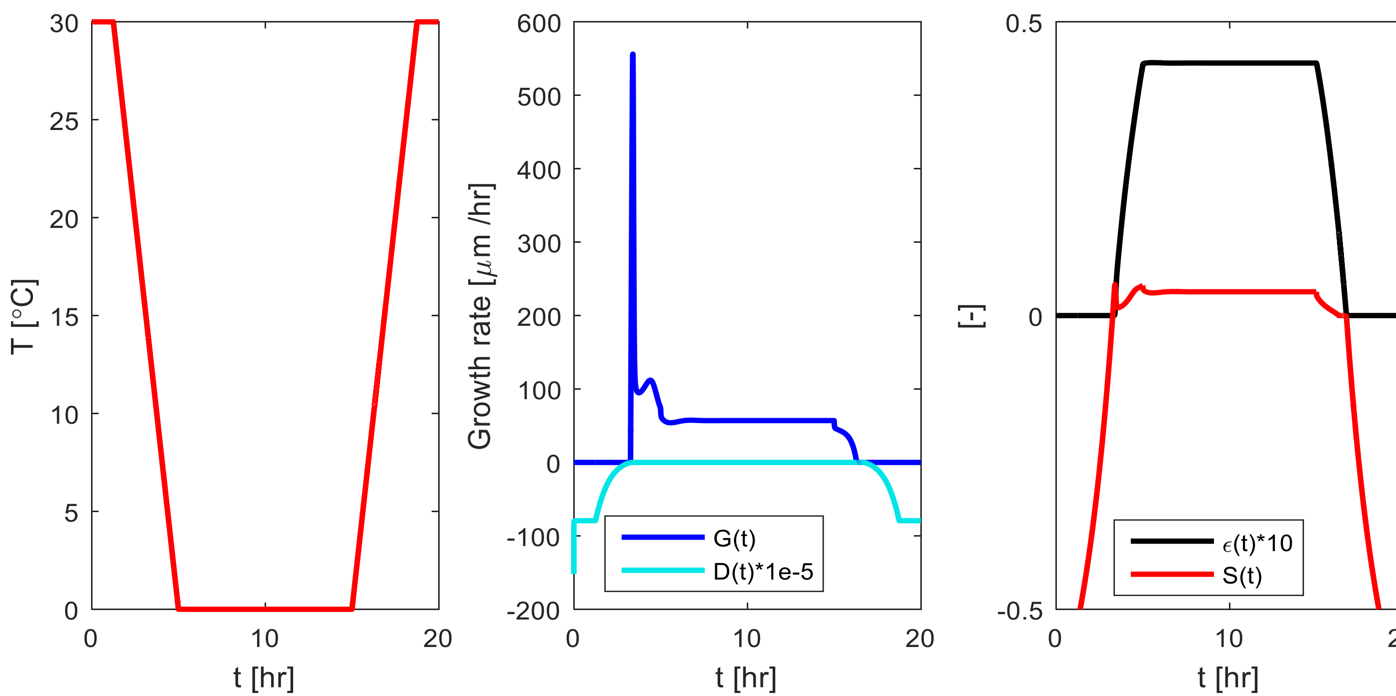
- Switching between regimes of positive and negative super-saturation:



S(t) - super - saturation

ε(t) - volume fraction of solid

$T(t) = mid\left(30, 0, -40 + \left|-80 + 8t\right|\right)$

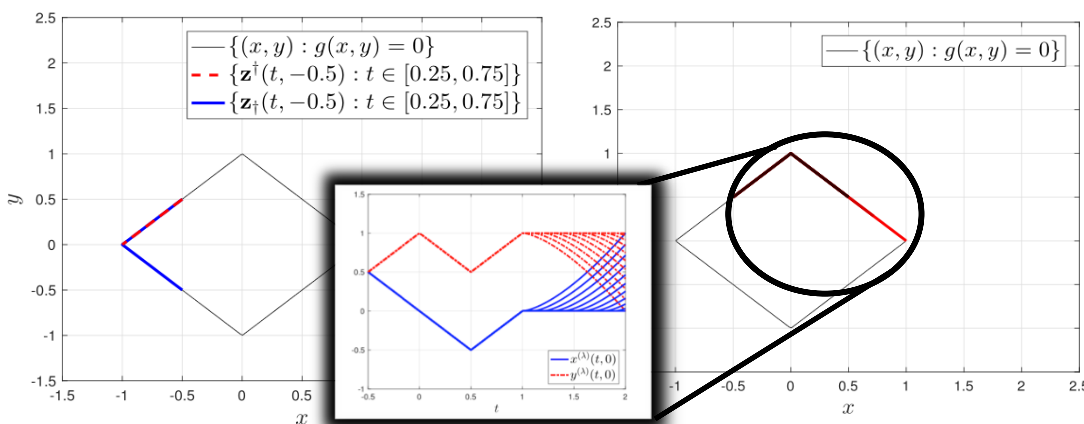


Regularization of Nonsmooth DAEs

- Nonsmooth DAEs:

$$\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$
$$\mathbf{0} = \mathbf{g}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$
$$\mathbf{x}(t_0,\mathbf{p}) = \mathbf{f}_0(\mathbf{p})$$

  - $\mathbf{f}$ is piecewise continuous w.r.t. t and continuous w.r.t. $\mathbf{p}, \mathbf{x}, \mathbf{y}$
  - $\mathbf{g}$ is locally Lipschitz continuous
  - "Index 1" Nonsmooth DAEs: generalized differentiation index one
  - Existence, uniqueness, continuous/Lipschitz dependence on parameters, etc.



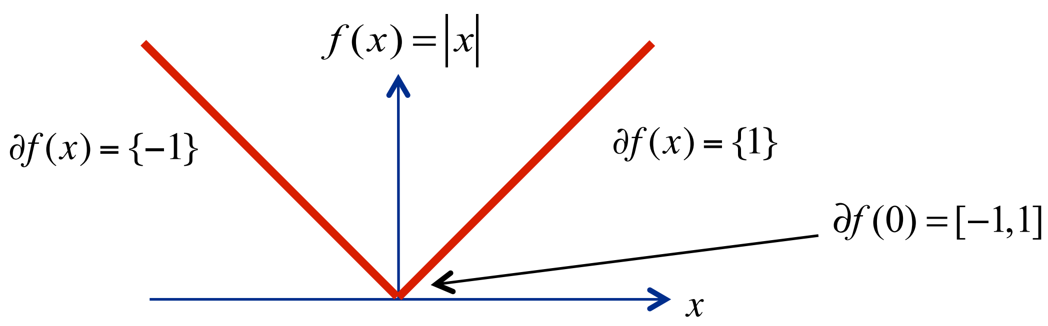
Stechlinski and Barton, *Journal Diff. Eqns.* 262 (2017): 2254–2285

Generalized Differentiation Index

- Given locally Lipschitz continuous $\mathbf{f}:\mathbb{R}^n \to \mathbb{R}^m$:
  - Clarke's Generalized Jacobian

$$\partial \mathbf{f}(\mathbf{x}) := \operatorname{conv}\left\{\mathbf{H} : \mathbf{Jf}(\mathbf{x}_{(j)}) \to \mathbf{H}, \mathbf{x}_{(j)} \to \mathbf{x}, \mathbf{x}_{(j)} \in X \setminus Z_{\mathbf{f}}\right\}$$

  - Example:



  - "Index-1" Nonsmooth DAE:

    No singular matrix in the set $\{\mathbf{M} : \exists[\mathbf{N}\ \ \mathbf{M}] \in \partial \mathbf{g}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))\}$
    - If $\mathbf{g}$ is C^1: $\left\{\frac{\partial \mathbf{g}}{\partial \mathbf{y}}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))\right\}$

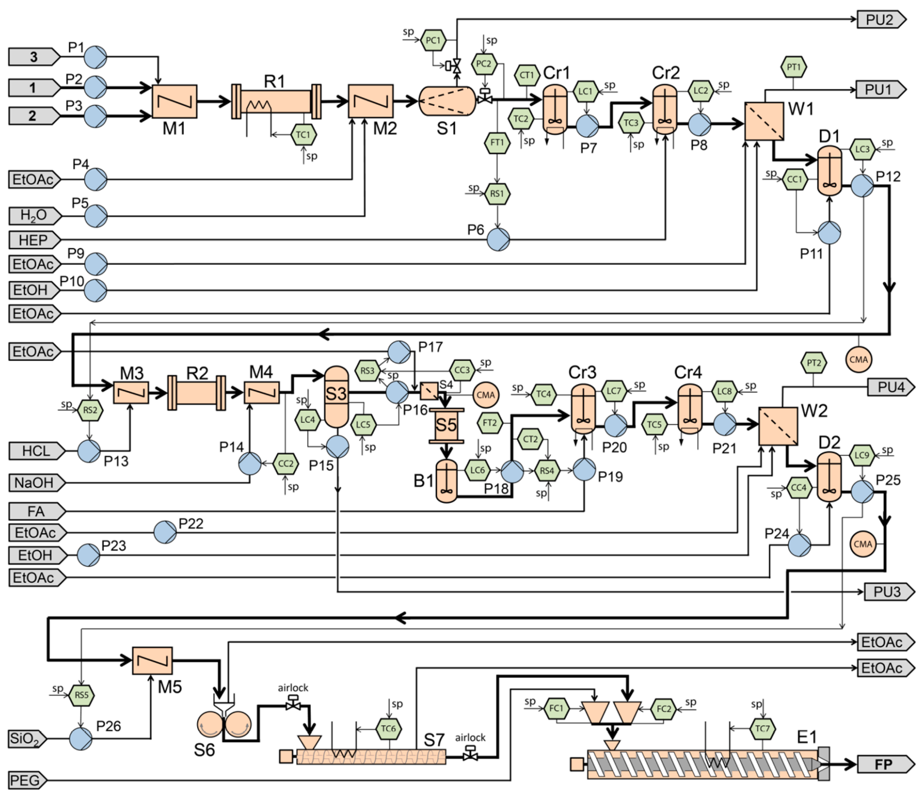
Clarke, Optimization and Nonsmooth Analysis, SIAM, 1990.
Stechlinski and Barton, *Journal Diff. Eqns.* 262 (2017): 2254–2285

The "Red-line"
Novartis-MIT Center

Mascia et al. "End-to-End Continuous Manufacturing of Pharmaceuticals: Integrated Synthesis, Purification, and Final Dosage Formation", *Angew. Chem. Int. Ed.* 2013, 52, 12359 –12363

Dynamic Optimization in PSE

- Campaign continuous manufacturing:
  - Maximize production, minimize off-spec.
  - "Discrete" phenomena: start-up/shut-down, phase changes, crystal growth/dissolution, etc., etc.



Sahlodin and Barton, *Ind. Eng. Chem. Res.* 54 (2015):11344-11359.

Dynamic Optimization of DAEs

- In the smooth case:

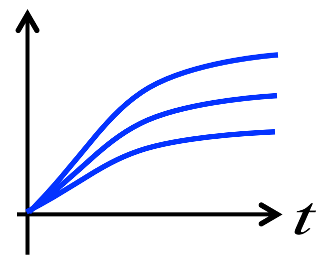
  - Semi-explicit index-1 DAE IVP

$$\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$
$$\mathbf{0} = \mathbf{g}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$
$$\mathbf{x}(t_0,\mathbf{p}) = \mathbf{f}_0(\mathbf{p})$$

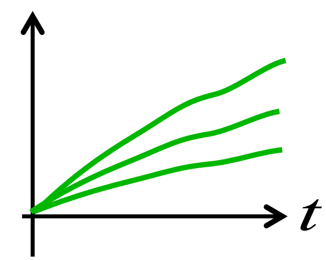
  - Sensitivity DAEs

$$\frac{\partial \dot{\mathbf{x}}}{\partial \mathbf{p}} = \frac{\partial \mathbf{f}}{\partial \mathbf{p}} + \frac{\partial \mathbf{f}}{\partial \mathbf{x}}\frac{\partial \mathbf{x}}{\partial \mathbf{p}} + \frac{\partial \mathbf{f}}{\partial \mathbf{y}}\frac{\partial \mathbf{y}}{\partial \mathbf{p}}$$
$$\mathbf{0} = \frac{\partial \mathbf{g}}{\partial \mathbf{p}} + \frac{\partial \mathbf{g}}{\partial \mathbf{x}}\frac{\partial \mathbf{x}}{\partial \mathbf{p}} + \frac{\partial \mathbf{g}}{\partial \mathbf{y}}\frac{\partial \mathbf{y}}{\partial \mathbf{p}}$$
$$\frac{\partial \mathbf{x}}{\partial \mathbf{p}}(t_0) = \mathbf{J}\mathbf{f}_0(\mathbf{p}_0)$$

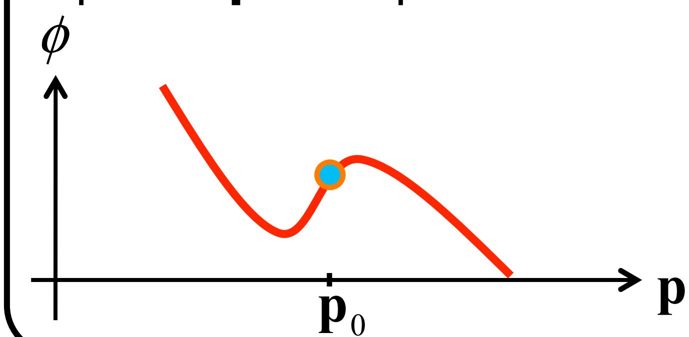
$\mathbf{x}(t,\mathbf{p}_0),\mathbf{y}(t,\mathbf{p}_0)$



$\frac{\partial \mathbf{x}}{\partial \mathbf{p}},\frac{\partial \mathbf{y}}{\partial \mathbf{p}}$



Update **p** via optimization



Dynamic Optimization of DAEs

- In the nonsmooth case:

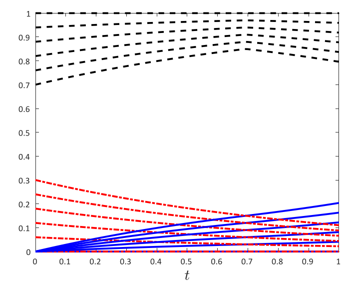
  - Semi-explicit "index-1" DAE IVP

$$\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$
$$\mathbf{0} = \mathbf{g}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$
$$\mathbf{x}(t_0,\mathbf{p}) = \mathbf{f}_0(\mathbf{p})$$

  - Nonsmooth sensitivity DAEs

???

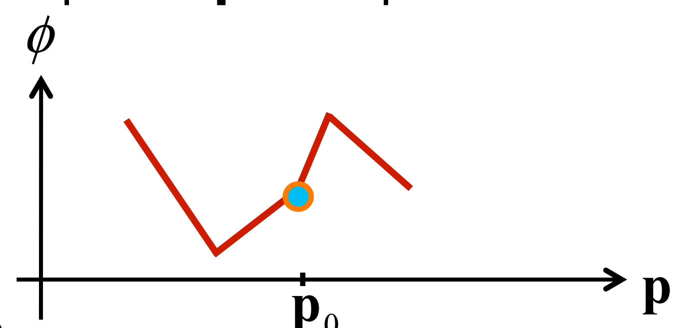
$\mathbf{x}(t,\mathbf{p}_0),\mathbf{y}(t,\mathbf{p}_0)$



$\dfrac{\partial \mathbf{x}}{\partial \mathbf{p}},\dfrac{\partial \mathbf{y}}{\partial \mathbf{p}}$

???

Update **p** via optimization

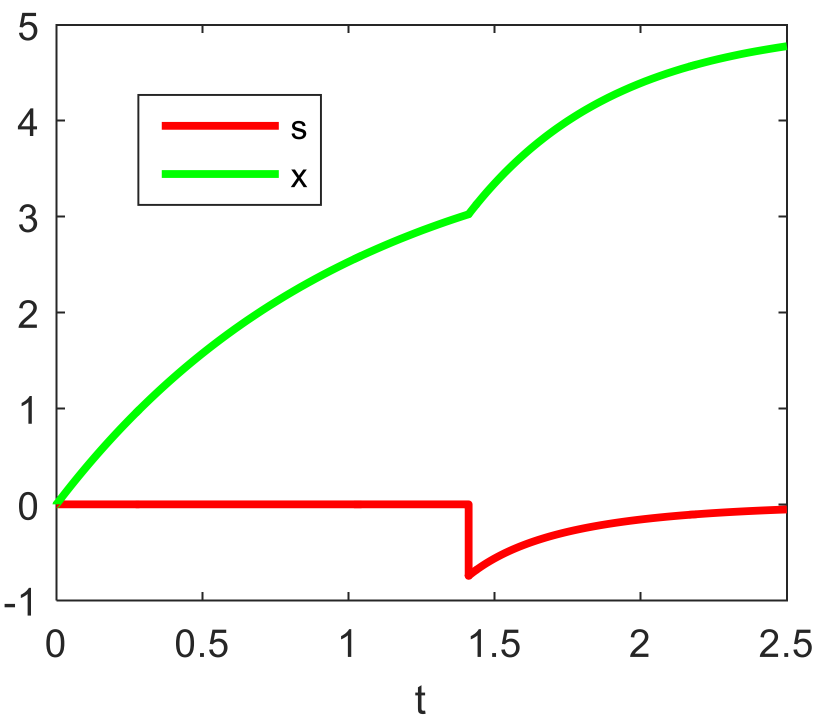


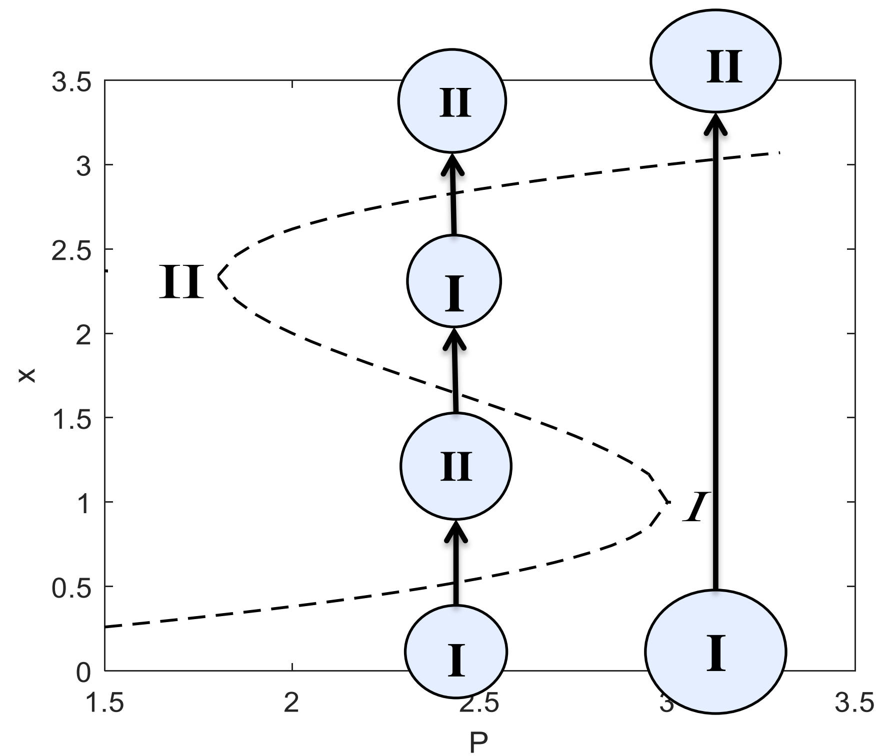
Sensitivities of Hybrid Automata

$$\dot{\mathbf{x}}^{(k)} = \mathbf{f}^{(k)}(t, \mathbf{p}, \mathbf{x}^{(k)}), \quad \mathbf{S}^{(k)} \equiv \frac{\partial \mathbf{x}^{(k)}}{\partial \mathbf{p}}$$

Transversality: $\frac{\partial g^{(k)}}{\partial \mathbf{x}^{(k)}} \dot{\mathbf{x}}^{(k)} \neq 0$

$$\mathbf{S}^{(k+1)} - \mathbf{S}^{(k)} = -\left[\mathbf{f}^{(k+1)} - \mathbf{f}^{(k)} \right] \frac{\partial t}{\partial \mathbf{p}}$$





Galan, Feehery, Barton, *App. Num. Math.* 31 (1999): 17-47

Nonsmooth DAE Sensitivities: Generalized Derivatives

- Want generalized derivative elements $\partial \mathbf{x}_{t_f}(\mathbf{p}_0), \partial \mathbf{y}_{t_f}(\mathbf{p}_0)$
  - Nonsmooth analog of $\frac{\partial \mathbf{x}}{\partial \mathbf{p}}(t_f, \mathbf{p}_0), \frac{\partial \mathbf{y}}{\partial \mathbf{p}}(t_f, \mathbf{p}_0)$
  - Difficult to evaluate in general (lack of sharp calculus rules, etc.)

- New tool: lexicographic directional (LD-)derivatives
  - Nonsmooth analog to classical directional derivative
  - Applicable to a wide class of functions (C^1, PC^1, convex, arbitrary compositions of such, etc.)
  - Satisfies strict calculus rules (e.g. chain rule)
  - Accurate, automatable and computationally cheap method

Khan and Barton, *Opt. Meth. & Soft.* 30 (2015): 1185-1212

Lexicographic Differentiation

- $\mathbf{f}: X \in \mathbf{R}^n \to \mathbf{R}^m$ is L-smooth at $\mathbf{x} \in X$ if it is locally Lipschitz continuous and directionally differentiable, and if, for any $\mathbf{M} := [\mathbf{m}_{(1)} \ \cdots \ \mathbf{m}_{(p)}] \in \mathbf{R}^{n \times p}$, the following functions exist:

$$\mathbf{f}_{\mathbf{x},\mathbf{M}}^{(0)} : \mathbf{d} \mapsto \mathbf{f}'(\mathbf{x};\mathbf{d})$$

$$\mathbf{f}_{\mathbf{x},\mathbf{M}}^{(1)} : \mathbf{d} \mapsto [\mathbf{f}_{\mathbf{x},\mathbf{M}}^{(0)}]'(\mathbf{m}_{(1)};\mathbf{d})$$

$$\vdots$$

$$\mathbf{f}_{\mathbf{x},\mathbf{M}}^{(p)} : \mathbf{d} \mapsto [\mathbf{f}_{\mathbf{x},\mathbf{M}}^{(p-1)}]'(\mathbf{m}_{(p)};\mathbf{d})$$

- If the columns of $\mathbf{M}$ span $\mathbf{R}^n$, then $\mathbf{f}_{\mathbf{x},\mathbf{M}}^{(p)}$ is linear, L-derivative:

$$\mathbf{J}_{\mathrm{L}}\mathbf{f}(\mathbf{x};\mathbf{M}) := \mathbf{J}\mathbf{f}_{\mathbf{x},\mathbf{M}}^{(p)}(\mathbf{0})$$

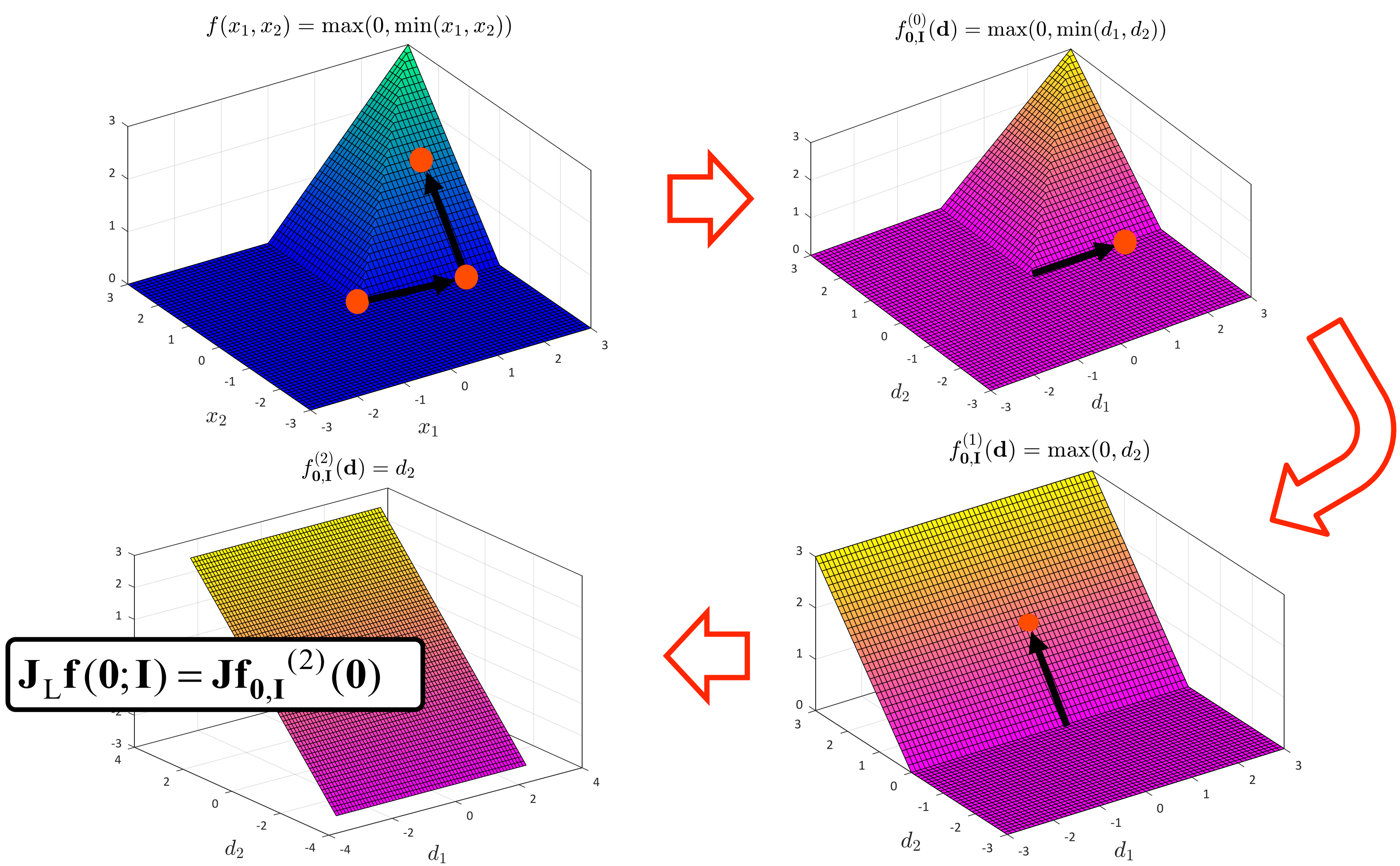
- Lexicographic subdifferential:

$$\partial_{\mathrm{L}}\mathbf{f}(\mathbf{x}) = \{\mathbf{J}_{\mathrm{L}}\mathbf{f}(\mathbf{x};\mathbf{M}) : \mathbf{M} \in \mathbf{R}^{n \times n},\ \det \mathbf{M} \neq 0\}$$

Y. Nesterov, *Math. Program. B*, 104 (2005) 669-700.

Lexicographic Differentiation

- Systematically probes local derivative information



LD-Derivatives

- Given L-smooth **f** and directions matrix $\mathbf{M} := \begin{bmatrix} \mathbf{m}_{(1)} & \cdots & \mathbf{m}_{(k)} \end{bmatrix}$

$$\mathbf{f}'(\mathbf{x};\mathbf{M}) := \begin{bmatrix} \mathbf{f}^{(0)}_{\mathbf{x},\mathbf{M}}(\mathbf{m}_{(1)}) & \mathbf{f}^{(1)}_{\mathbf{x},\mathbf{M}}(\mathbf{m}_{(2)}) & \cdots & \mathbf{f}^{(k-1)}_{\mathbf{x},\mathbf{M}}(\mathbf{m}_{(k)}) \end{bmatrix}$$

- If **M** is square and nonsingular: $\mathbf{f}'(\mathbf{x};\mathbf{M}) = \mathbf{J}_{\mathrm{L}}\mathbf{f}(\mathbf{x};\mathbf{M})\mathbf{M}$

- If **f** is C¹ at **x**: $\mathbf{f}'(\mathbf{x};\mathbf{M}) = \mathbf{J}\mathbf{f}(\mathbf{x})\mathbf{M}$

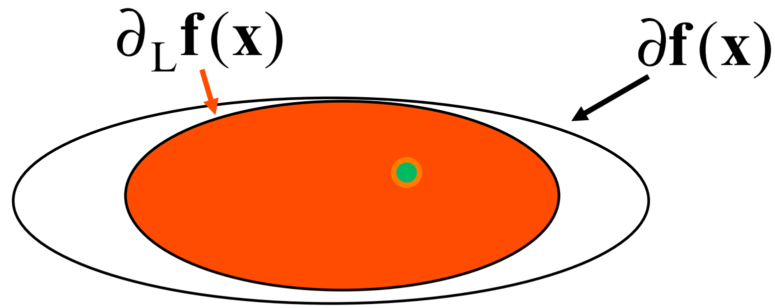
- Sharp LD-derivative chain rule:

$$\left[\mathbf{f}\circ\mathbf{g}\right]'(\mathbf{x};\mathbf{M}) = \mathbf{f}'(\mathbf{g}(\mathbf{x});\mathbf{g}'(\mathbf{x};\mathbf{M}))$$

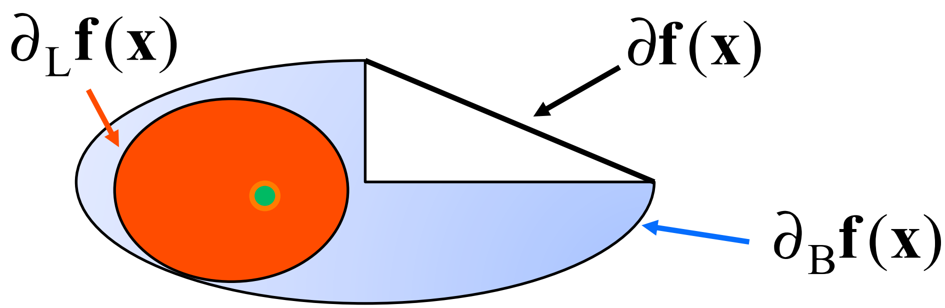
Khan and Barton, *Opt. Meth. & Soft.* 30 (2015): 1185-1212

Generalized Derivatives Landscape

- Given $\mathbf{f}:\mathbf{R}^n \rightarrow \mathbf{R}^m$
  - If m=1 (e.g., objective function):



  - If **f** is PC[1]:



  - If **f** is C[1]: $\longleftarrow \partial_L \mathbf{f}(\mathbf{x}) = \partial_B \mathbf{f}(\mathbf{x}) = \partial \mathbf{f}(\mathbf{x}) = \{\mathbf{Jf}(\mathbf{x})\}$

- LD-derivatives furnish gen. deriv. elements (green dots) in tractable way

Khan and Barton, *Opt. Meth. & Soft.* 30 (2015): 1185-1212
Khan and Barton, *Journal Opt. Theory. Appl.* 163 (2014): 355-386

Dynamic Optimization of DAEs

- In the nonsmooth case:

  - Semi-explicit "index-1" DAE IVP

$$\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$
$$\mathbf{0} = \mathbf{g}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p}),\mathbf{y}(t,\mathbf{p}))$$
$$\mathbf{x}(t_0,\mathbf{p}) = \mathbf{f}_0(\mathbf{p})$$

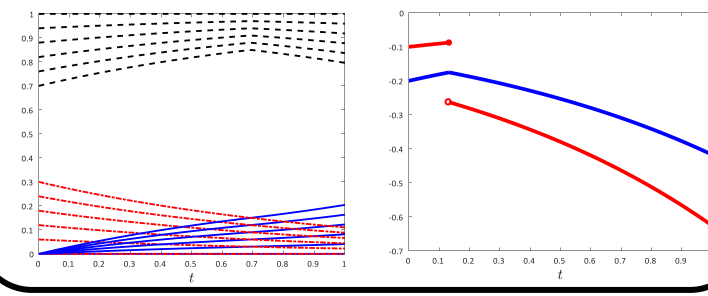
  - Nonsmooth sensitivities DAEs

$$\dot{\mathbf{X}}(t) = [\mathbf{f}_t]'(\mathbf{p}_0,\mathbf{z}(t,\mathbf{p}_0);(\mathbf{M},\mathbf{Z}(t)))$$
$$\mathbf{0} = [\mathbf{g}_t]'(\mathbf{p}_0,\mathbf{z}(t,\mathbf{p}_0);(\mathbf{M},\mathbf{Z}(t)))$$
$$\mathbf{X}(t_0) = [\mathbf{f}_0]'(\mathbf{p}_0;\mathbf{M})$$

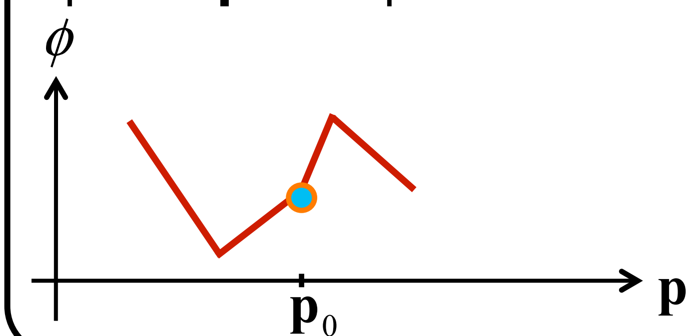
where

$$\mathbf{z} \equiv (\mathbf{x},\mathbf{y}), \mathbf{Z} \equiv (\mathbf{X},\mathbf{Y}) \equiv [\mathbf{z}_t]'(\mathbf{p}_0;\mathbf{M})$$

$\mathbf{x}(t,\mathbf{p}_0)$, $\mathbf{y}(t,\mathbf{p}_0)$ $\quad$ $\mathbf{J}_L\mathbf{x}_t(\mathbf{p}_0;\mathbf{M})$, $\mathbf{J}_L\mathbf{y}_t(\mathbf{p}_0;\mathbf{M})$



Update **p** via optimization

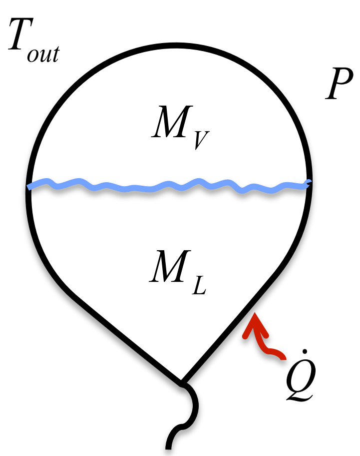


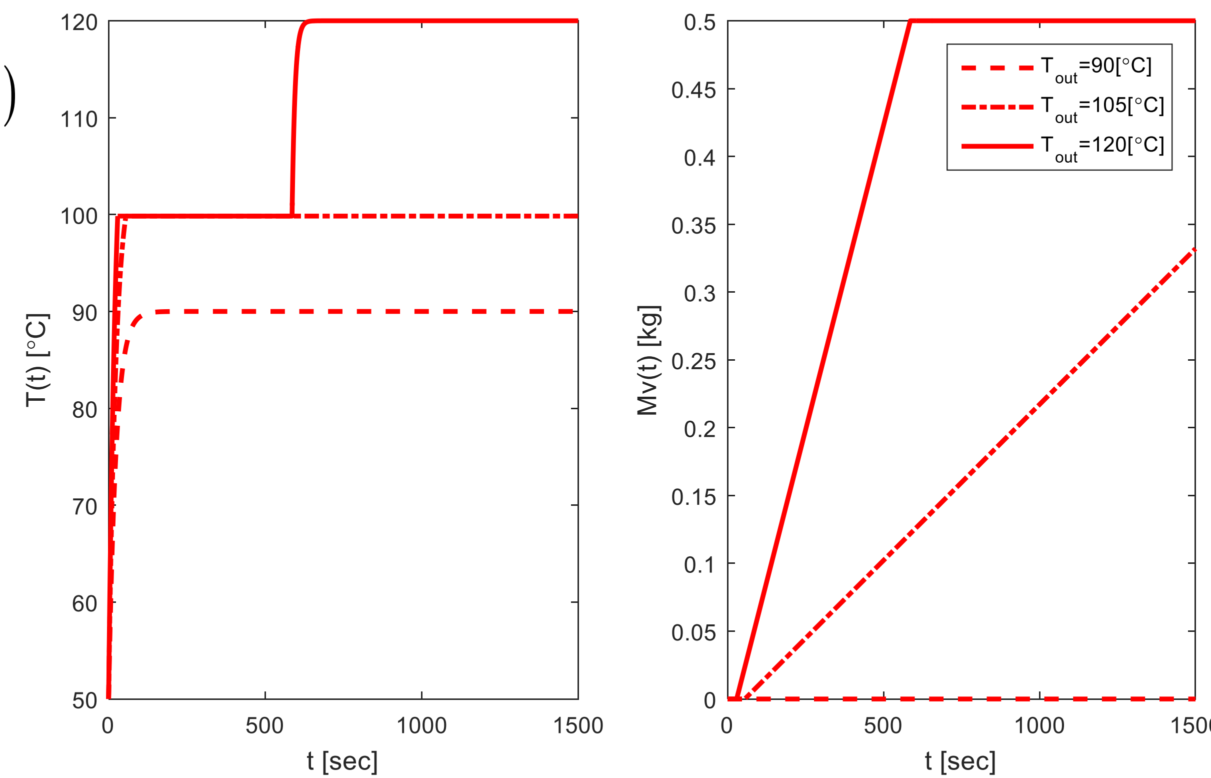
Simple Flash Process: Mode Sequence

- Mode sequence varies under parametric perturbations

$$\dot{H}(t) = U\left(T_{out} - T(t)\right)$$
$$M = M_L(t) + M_V(t)$$
$$H(t) = Mh_V(t) - M_L(t)\Delta h_{vap}\left(T(t)\right)$$
$$h_V(t) = Cp\left(T(t) - T_0\right)$$
$$\log\left(P^{sat}(t)\right) = A - B / \left(T(t) + C\right)$$

+ hybrid automaton

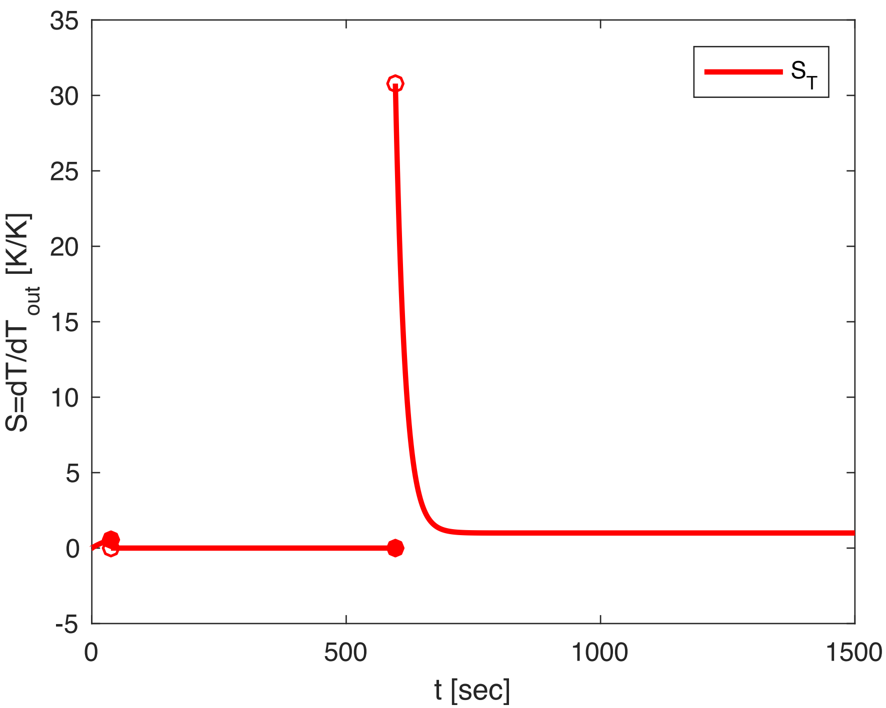


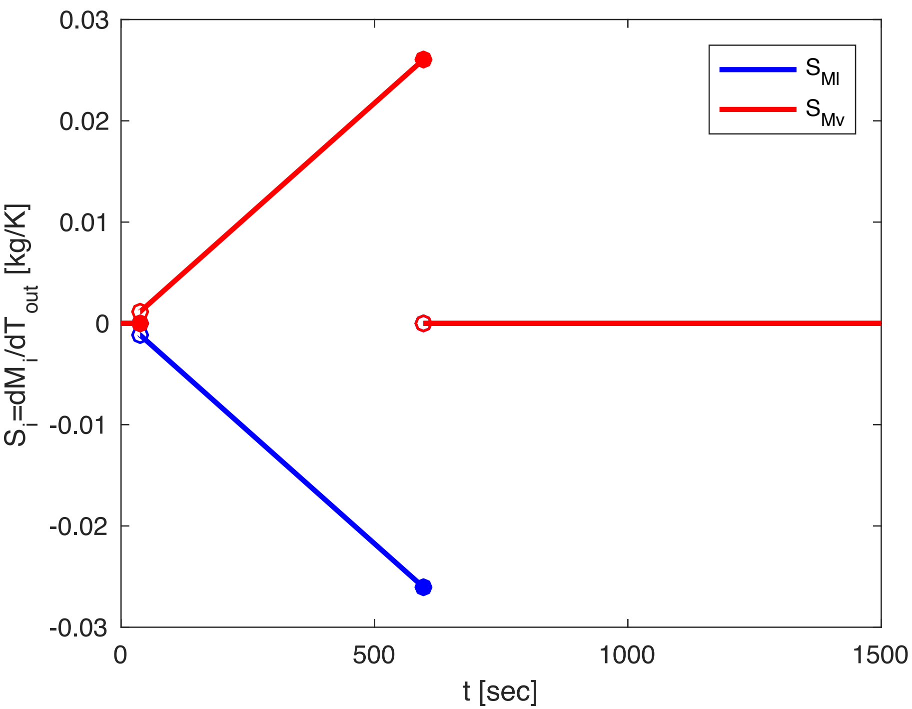


Simple Flash Process: Sensitivities

- Nonsmooth sensitivities:

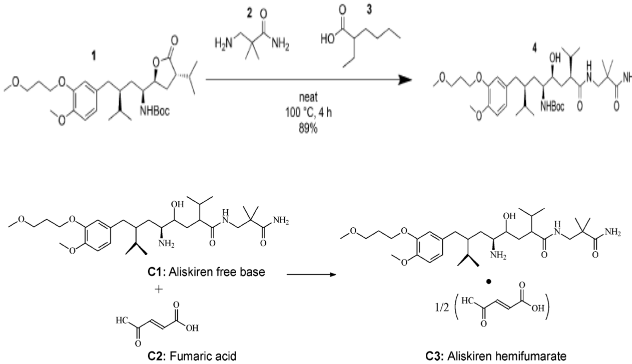
$$\dot{S}_H(t) = U\left(1 - S_T(t)\right)$$
$$S_H(t) = MCpS_T(t) - \Delta h_{vap}'\left(T(t)\right)S_T(t)$$
$$0 = \text{mid}'\left(M_V(t), P - P_{sat}\left(T(t)\right), -M_L(t); (S_V(t), -P_{\text{sat}}'(T(t))S_T(t), -S_L(t))\right)$$
$$S_V(t) = -S_L(t)$$



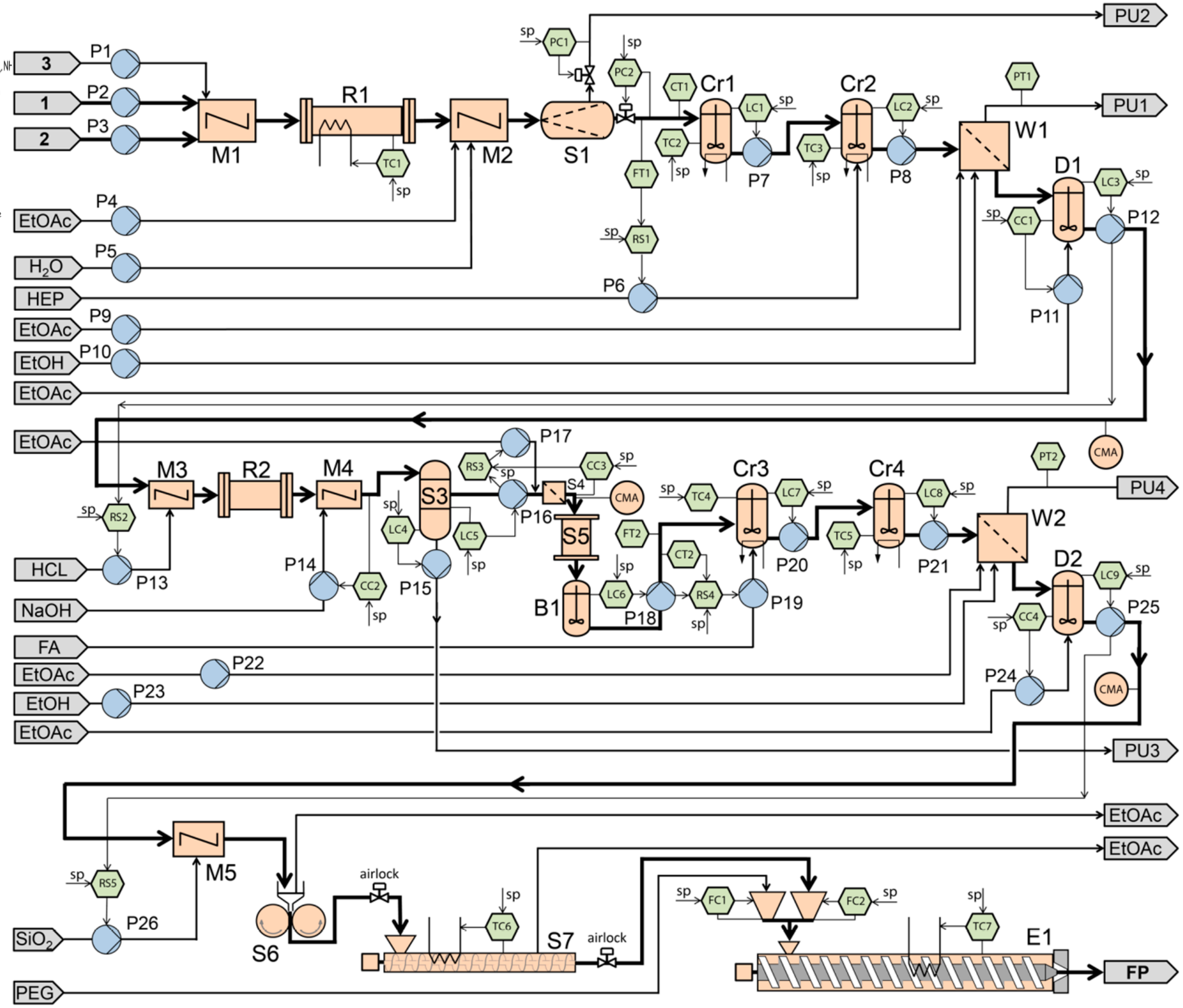


No Notion of Mode Sequence Needed

The “Red-line” Process Flow Diagram



Unit operation[a]	t [h]
R1	4
S1	< 0.1
Cr1 + Cr2	8
W1	< 0.1
D1	2
R2	< 0.1
S3	2
S5	15
Cr3 + Cr4	8
W2	< 0.1
D2	2
S6 + S7	6
E1	< 0.1
MD	< 0.1
Total	47



R. Lakerveld et. al, “The Application of an Automated Control Strategy for an Integrated Continuous Pharmaceutical Pilot Plant”, Org. Process Res. Dev. 2015, 19, 1088−1100.

The "Red-line" Nonsmooth Process Model

No hold-up Liquid-Liquid-Equilibrium:

$$mid\left(\frac{F^{raf}}{F^{raf}+F^{pur})}-1, \sum_{i=1}^{nc} w_i^{pur1}-\sum_{i=1}^{nc} w_i^{raf1}, \frac{F^{raf1}}{F^{raf1}+F^{pur1}}\right)=0$$

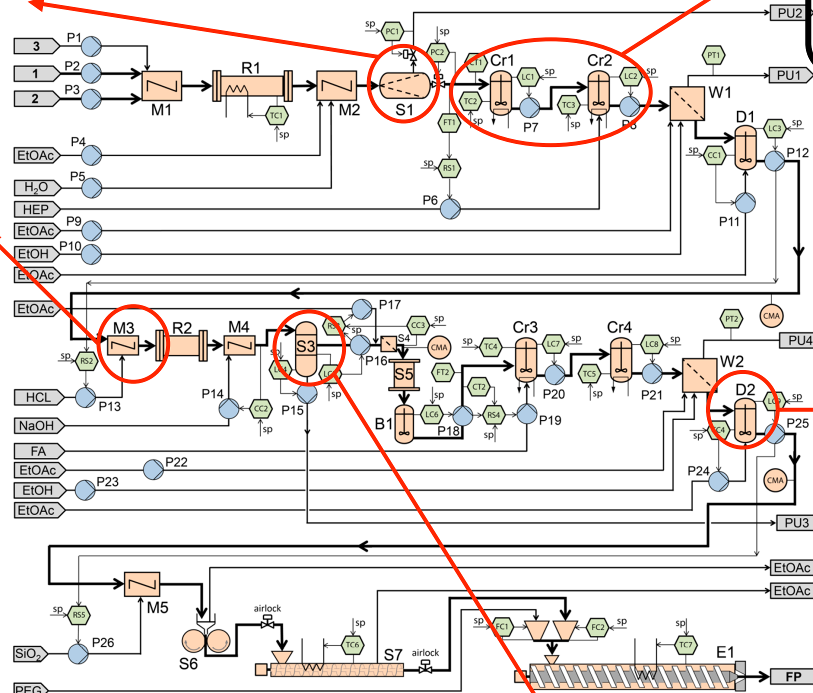
Crystallization kinetics:

$$G(t)=\max\left(0, k_G S(t)\left|S(t)\right|^{n_G-1}\right)$$

$$D(t)=\min\left(k_D S(t)\left|S(t)\right|^{n_D-1}, 0\right)$$

Flow set point for dilution:

$$F_{S_1}=max\left(\frac{F^{raf}w_C^{raf}}{w^{s.p}}-F^{raf}, 0\right)$$



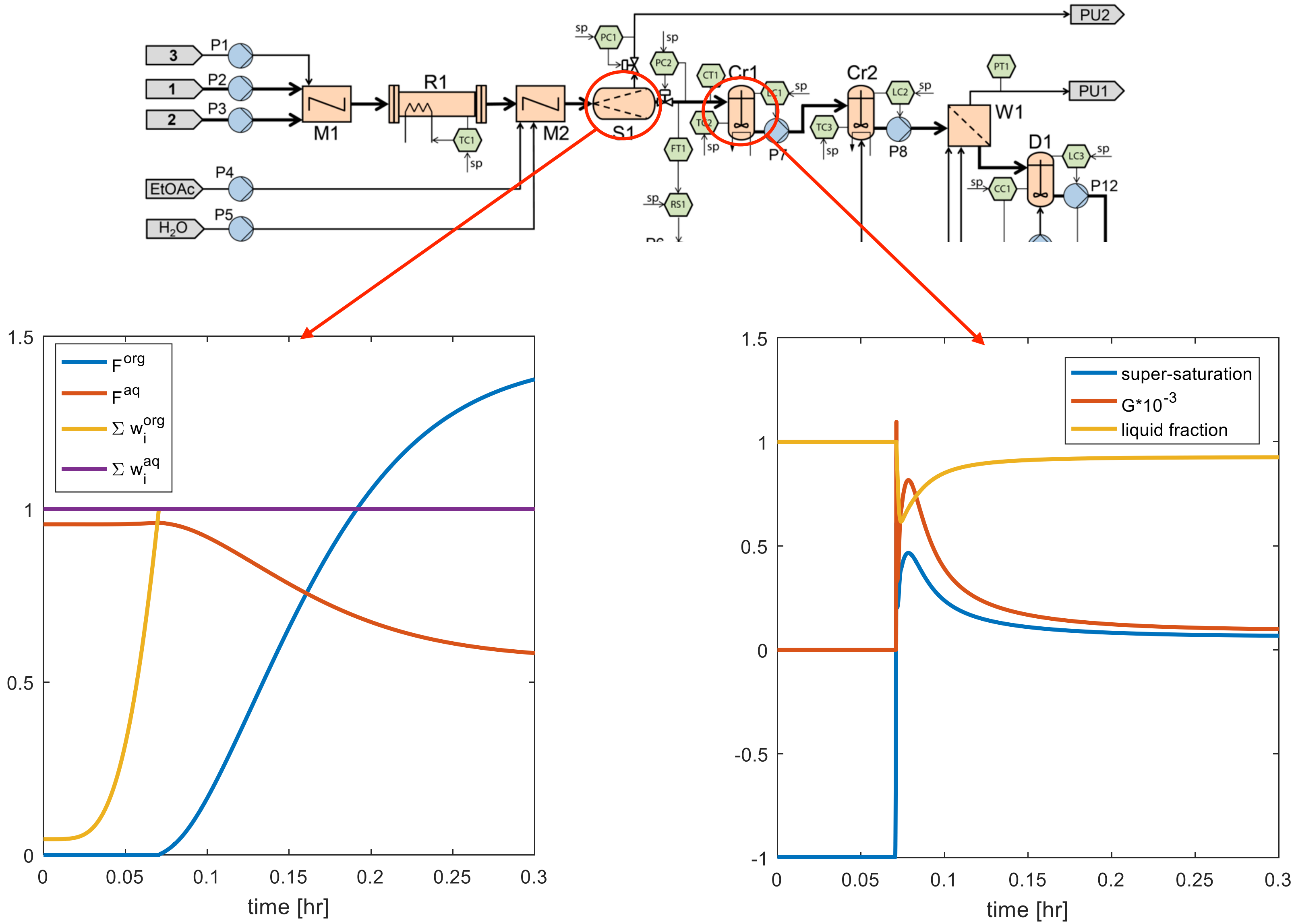
Valves (weirs):

$$F_{out}=\max\left(0, u(t)\frac{V^{Cr1}-V_{min}}{\sqrt{|V^{Cr1}-V_{min}|+\varepsilon}}\right)$$

Dynamic Liquid-Liquid-Equilibrium with hold-ups:

$$mid\left(\frac{M^{raf}}{M^{raf}+M^{pur}}-1, \sum_{i=1}^{nc} w_i^{pur}-\sum_{i=1}^{nc} w_i^{raf}, \frac{M^{raf}}{M^{raf2}+M^{pur3}}\right)=0$$

The "Red-line"
Nonsmooth Process Simulation



Dynamic Optimization:
Problem formulation

<u>Our approach, inspired by the 'turnpike theory':</u>

$$\max_{u, t^{on}, t^{off}} \int_{t^{on}}^{t^{off}} J = \text{objective function}$$

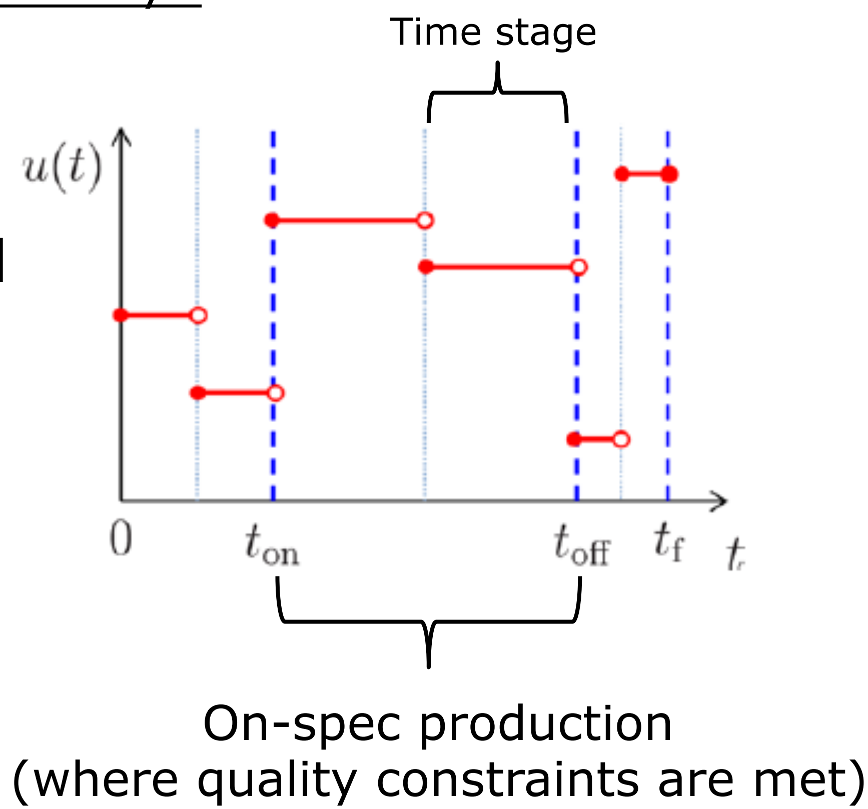
$$s.t. \quad \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{y}, \mathbf{u}, t), \quad \mathbf{x}(0) = \mathbf{x}_0, \quad t \in [0, t^{final}]$$

$$\mathbf{0} = \mathbf{g}(\mathbf{x}, \mathbf{y}, \mathbf{u}, t)$$

safety constraints $t \in [0, t^{final}]$

quality constraints $t \in [t^{on}, t^{off}]$

final time constraints $t = t^{final}$



<u>Comparison to the classical approach:</u>

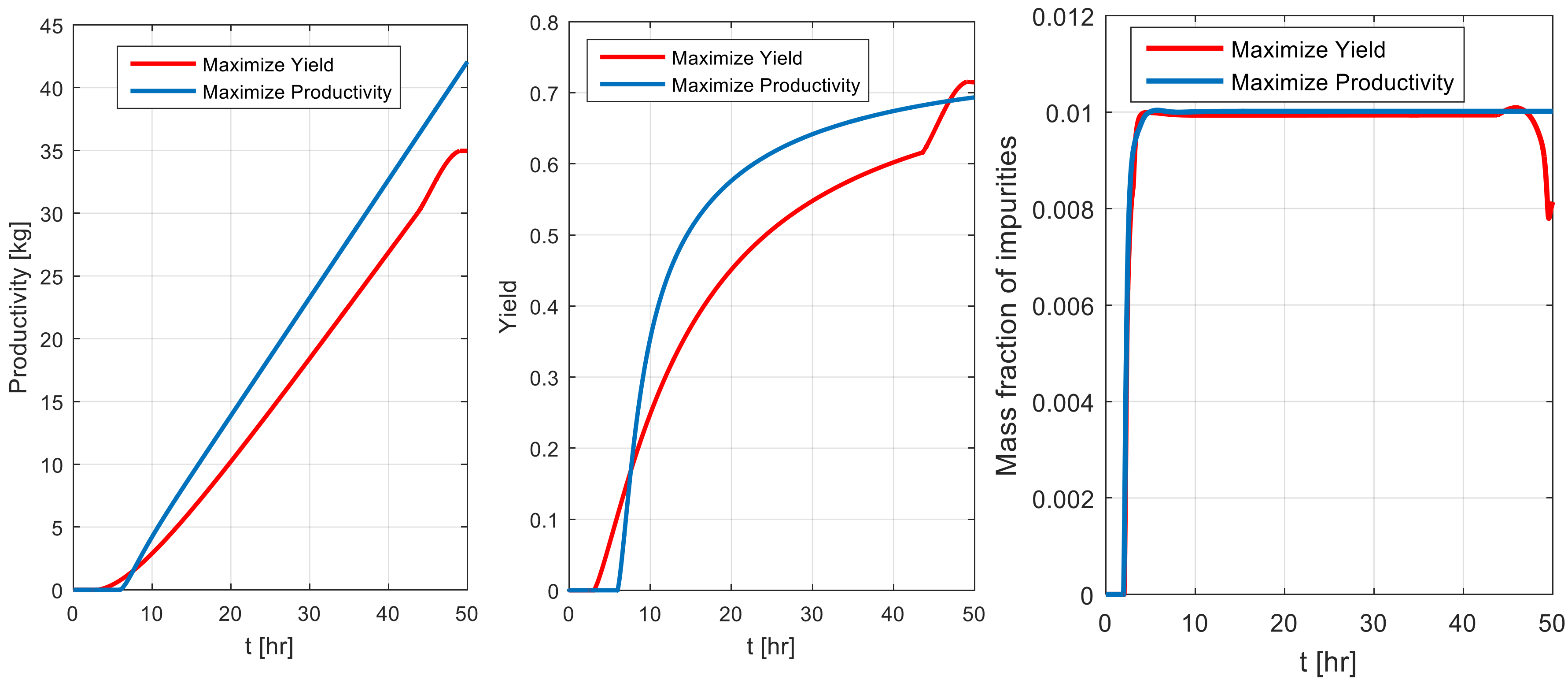
$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{y}, \mathbf{u}, t) = \mathbf{0}, \quad \forall t \in \left[t^{on}, t^{off}\right]$$

A. M. Sahlodin and P. I. Barton, Optimal Campaign Continuous Manufacturing
Ind. Eng. Chem. Res., 2015, 54 (45), pp 11344–11359

Case study: Multi Objective Optimization

$$\max \quad \text{Yield} = \frac{MW^{C1}}{MW^{P}} \int_{t_{on}}^{t_{off}} F^{P}_{on\text{-}spec} \Bigg/ \int_{0}^{t_f} F_{C1}$$

$$\max \quad \text{Productivity} = \int_{t_{on}}^{t_{off}} F^{P}_{on\text{-}spec}$$

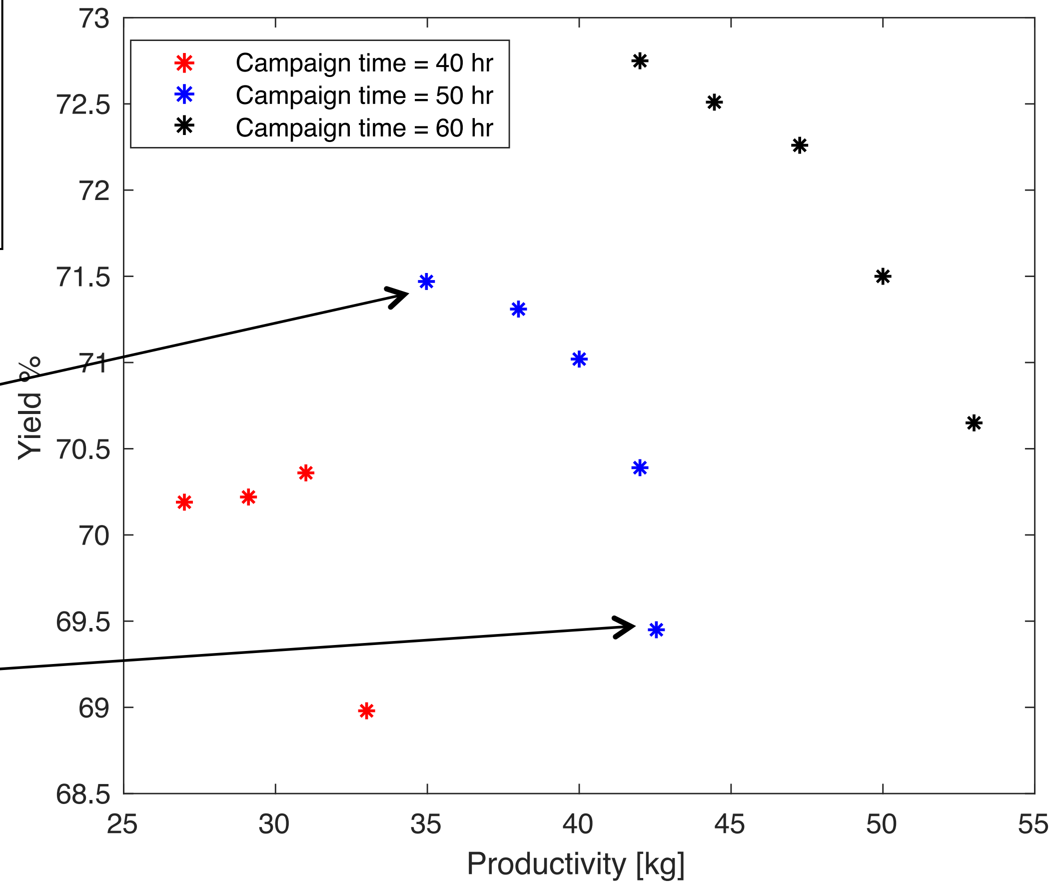


Case study: Pareto Curves

$$\max \quad Yield$$
$$s.t$$
$$\left.\begin{aligned} & x_P > 0.26 \\ & \sum x_I < 0.01 \end{aligned}\right\} \quad \text{quality constraints}$$
$$\int_{t_{on}}^{t_{off}} F^P_{on\text{-}spec} = M^P \quad \text{operational constraint}$$

Maximize yield

Maximize productivity



Nonsmooth DAEs

- Summary of Progress:
  - Possess a strong mathematical theory (recently)
    - Hence, formulate model this way if you can!
  - Easy-to-use and solve and do sensitivity analysis
  - Applicable to variety of operational problems:
    - See Sahlodin, Watson and Barton, *AIChE Journal* 62 (2016)
  - Numerical toolkit: amenable to computationally tractable (e.g. automatic differentiation) methods
    - See Khan and Barton, *OM&S* 30 (2015)
    - LD-derivative rules for abs, min, max, mid, 2-norm, etc.

- Future Work:
  - Numerical implementations
  - “High-index” nonsmooth DAEs
  - Adjoint sensitivities

Acknowledgments

- Peter Stechlinski, Michael Shoham Patrascu, Harry Watson, Kamil Khan, Ali Sahlodin
- Funding Sources:
  - The Novartis-MIT Center for Continuous Manufacturing
  - Natural Sciences and Engineering Research Council of Canada (NSERC)

NOVARTIS

NSERC
CRSNG

Flow Transitions

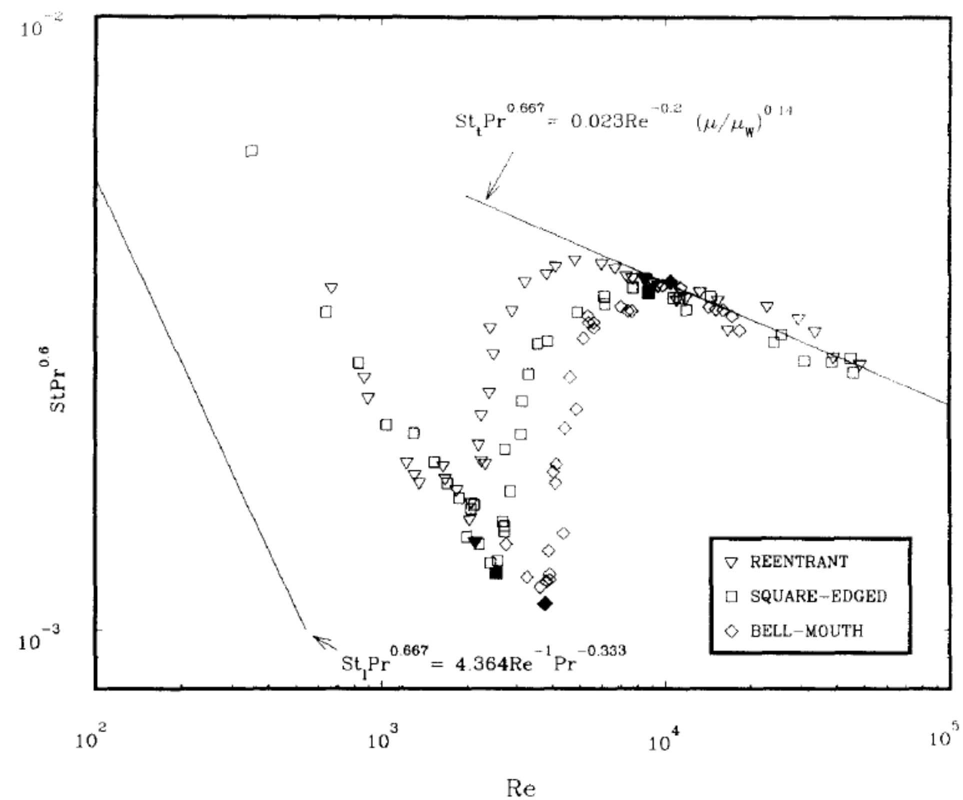
- Transitioning between flow regimes can be modeled using one nonsmooth equation

$$\mathrm{Nu}(t) = \max\left(\mathrm{Nu}_l(t), \mathrm{Nu}_{\mathrm{tr}}(t)\right)$$

$$\mathrm{Nu}_l(t) = 14.5$$

$$\mathrm{Nu}_{\mathrm{tr}}(t) = \left(\mathrm{Nu}_l \exp\left(\left(\mathrm{Re}(t) - \mathrm{Re}_c\right)/b\right) + \mathrm{Nu}_t^{\,c}\right)^c$$

$$\mathrm{Nu}_t(t) = 0.023\,\mathrm{Re}(t)^{0.8}\,\mathrm{Pr}^{1/3}$$



➢ Ghajar and Tam, *Exp. Therm. Fluid Sci*. 8 (1994): 79-90

Sensitivities of Nonsmooth DAEs

- DAE Smooth vs. Nonsmooth:
  - Nonsmooth sensitivities:

$$\dot{\mathbf{X}}(t) = [\mathbf{f}_t]'(\mathbf{p}_0, \mathbf{x}(t,\mathbf{p}_0), \mathbf{y}(t,\mathbf{p}_0); (\mathbf{M}, \mathbf{X}(t), \mathbf{Y}(t))$$
$$\mathbf{0} = [\mathbf{g}_t]'(\mathbf{p}_0, \mathbf{x}(t,\mathbf{p}_0), \mathbf{y}(t,\mathbf{p}_0); (\mathbf{M}, \mathbf{X}(t), \mathbf{Y}(t))$$
$$\mathbf{X}(t_0) = [\mathbf{f}_0]'(\mathbf{p}_0; \mathbf{M})$$

  - Nonsmooth and nonlinear DAE system
  - Unique solution and unique initialization
  - $\mathbf{X}$ continuous, $\mathbf{Y}$ discontinuous
  - Once solved, obtain generalized derivative elements (sensitivities) via linear equation solve

  - Smooth sensitivities:

$$\frac{\partial \dot{\mathbf{x}}}{\partial \mathbf{p}} = \frac{\partial \mathbf{f}}{\partial \mathbf{p}} + \frac{\partial \mathbf{f}}{\partial \mathbf{x}}\frac{\partial \mathbf{x}}{\partial \mathbf{p}} + \frac{\partial \mathbf{f}}{\partial \mathbf{y}}\frac{\partial \mathbf{y}}{\partial \mathbf{p}}$$
$$\mathbf{0} = \frac{\partial \mathbf{g}}{\partial \mathbf{p}} + \frac{\partial \mathbf{g}}{\partial \mathbf{x}}\frac{\partial \mathbf{x}}{\partial \mathbf{p}} + \frac{\partial \mathbf{g}}{\partial \mathbf{y}}\frac{\partial \mathbf{y}}{\partial \mathbf{p}}$$
$$\frac{\partial \mathbf{x}}{\partial \mathbf{p}}(t_0) = \mathbf{J}\mathbf{f}_0(\mathbf{p}_0)$$

  - Linear DAE system
  - Unique soln. & init.
  - $\frac{\partial \mathbf{x}}{\partial \mathbf{p}}(\cdot, \mathbf{p}_0), \frac{\partial \mathbf{y}}{\partial \mathbf{p}}(\cdot, \mathbf{p}_0)$ continuous

- Stechlinski and Barton, *Journal Opt. Theory. Appl.* 171 (2016): 1-26