# From Model-Based Open loop Optimization Strategies to Feedback-based Optimization via NCO Tracking


Dr. Grégory François

– Associate Professor, ELIAUS, UPVD

– *PhD, Laboratoire d'Automatique, Swiss Federal Institute of Technology, Lausanne, Switzerland*

– *BSc and MSc in Chemical Engineering (ENSIC-INPL, Nancy, France)*



GRD-MACS, Groupe de Travail CPNL

ENSAM, Paris, 05/06/2008

# Outline

- Introduction
- Dynamic Optimization of Batch Processes
- Measurement-Based Optimization via NCO-Tracking
  - Choice of Manipulated Variables: Solution Model
  - Tracking the Necessary Conditions of Optimality
- Ex: Run-to-Run Optimization (theory)
  - Influence of Uncertainty and Input Decoupling
  - Controller Structure and Convergence Analysis
- Application to Industrial Acrylamide Copolymerization
- Conclusion & Perspectives
- Bibliography

# Introduction

- Similarity between control and optimization methodologies.

- Exploit this synergy.
  - *Self-optimizing control structure: "The goal is to find a set of controlled variables which, when kept at constant setpoints, indirectly lead to near-optimal operation with acceptable loss.", S. Skogestad, NTNU Trondheim.*
  - *Early work on extremum-seeking control , revisited recently (Krstic, …)*

- Challenge = defining inputs, outputs, setpoints for feedback-based optimization

# Outline

- Introduction
- Dynamic Optimization of Batch Processes
  - Nominal Model-Based Optimization
  - Limitations of the Use of Dynamic Optimization in Industry
- Measurement-Based Optimization via NCO-Tracking
  - Choice of Manipulated Variables: Solution Model
  - Tracking the Necessary Conditions of Optimality
- Run-to-Run Optimization
  - Influence of Uncertainty and Input Decoupling
  - Controller Structure and Convergence Analysis
- Application to Industrial Acrylamide Copolymerization
- Conclusion & Perspectives

# Dynamic Optimization of Batch Processes

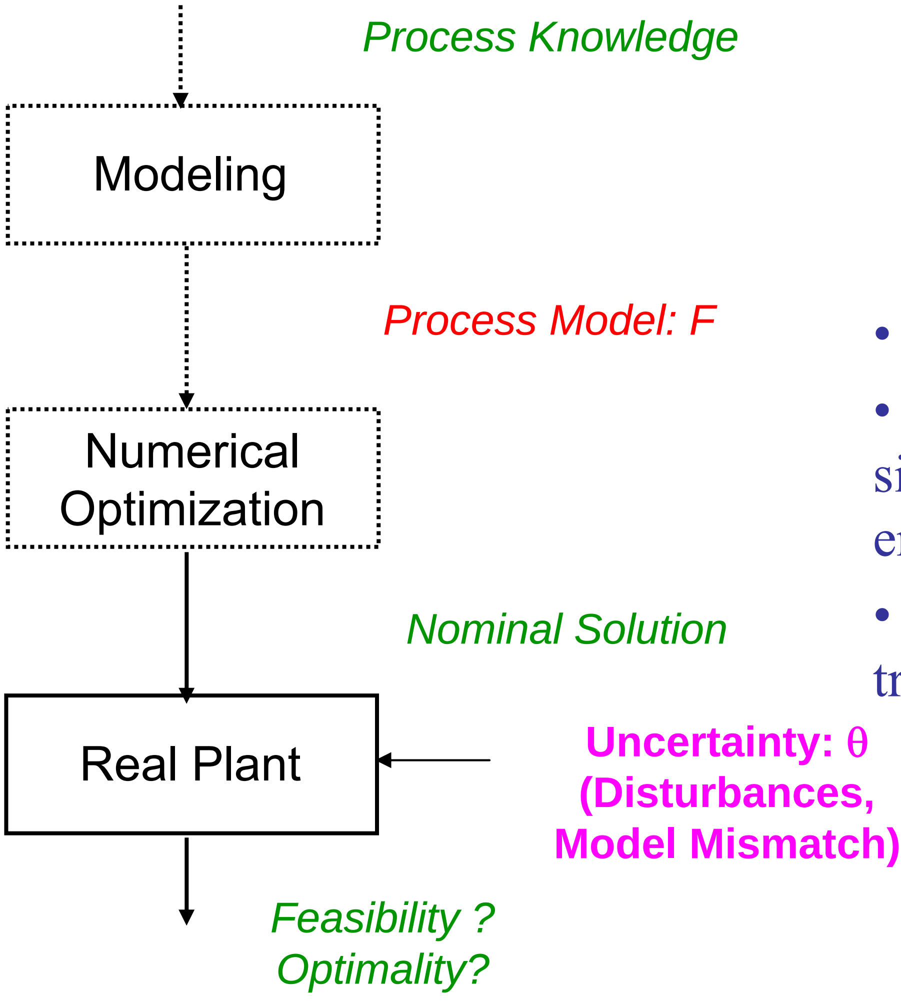
- Problem Formulation:
  - Determining the control profile that minimizes a pre-specified cost-function
  - Guaranteeing the respect of Path and Terminal Constraints

$$\min_{u(t),t_f} J = \phi\left(x(t_f)\right)$$

$$s.t.: \begin{cases} \dot{x}(t) = f\left(x(t), u(t), \theta\right) \\ S\left(x(t), u(t), \theta\right) \leq 0 \\ T\left(x(t_f), \theta\right) \leq 0 \end{cases}$$

- model mismatch
- uncertainties
- numerical difficulties

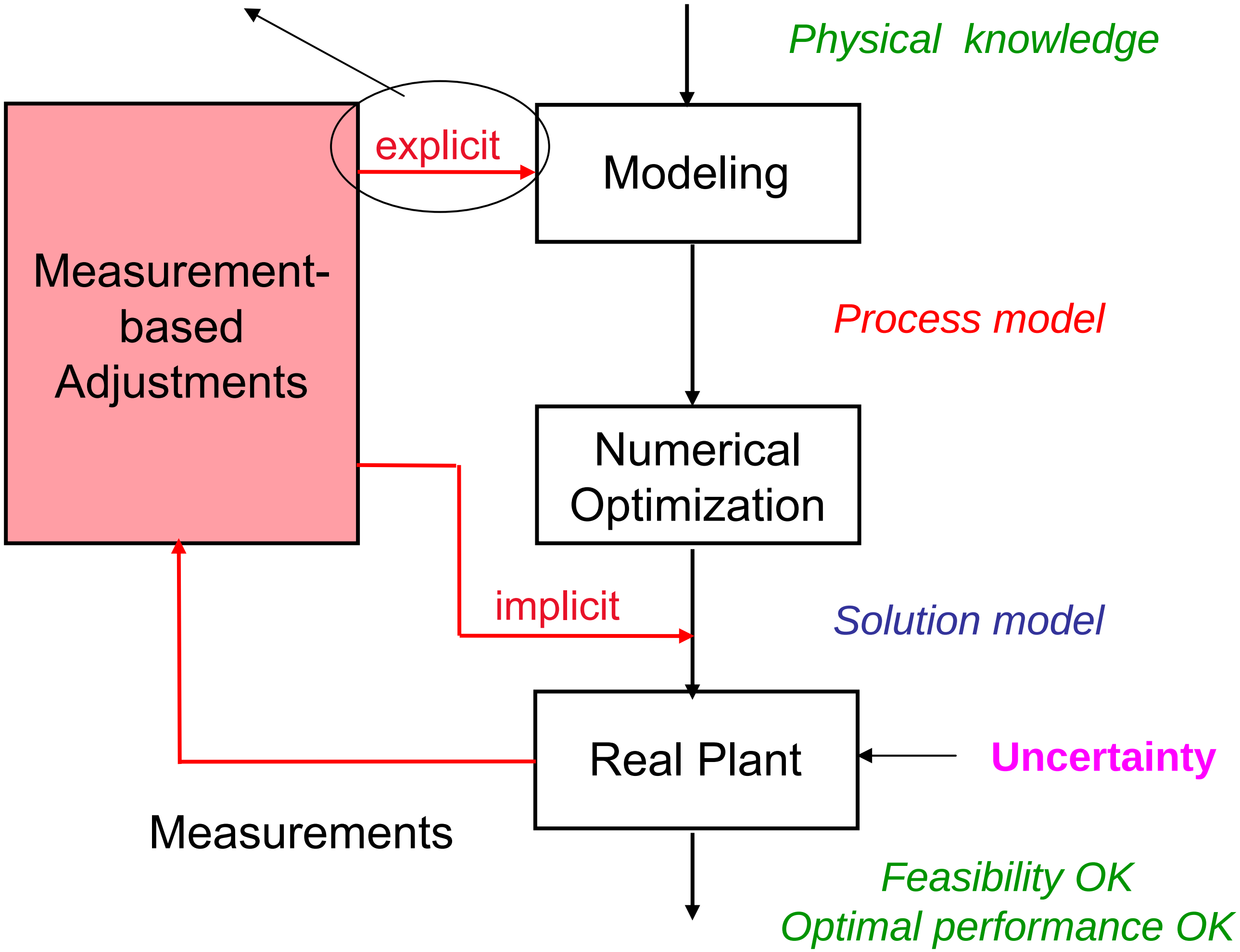
# Nominal Optimization




- = Open-loop strategies!
- MPC is not purely Open-loop since states are reinitialized at the end of the control Horizon
- How to "close the loop ?" (e.g. trajectory following)

# Measurement-Based Optimization

e.g. : model refinement



# Implicit Measurement-Based Optimization

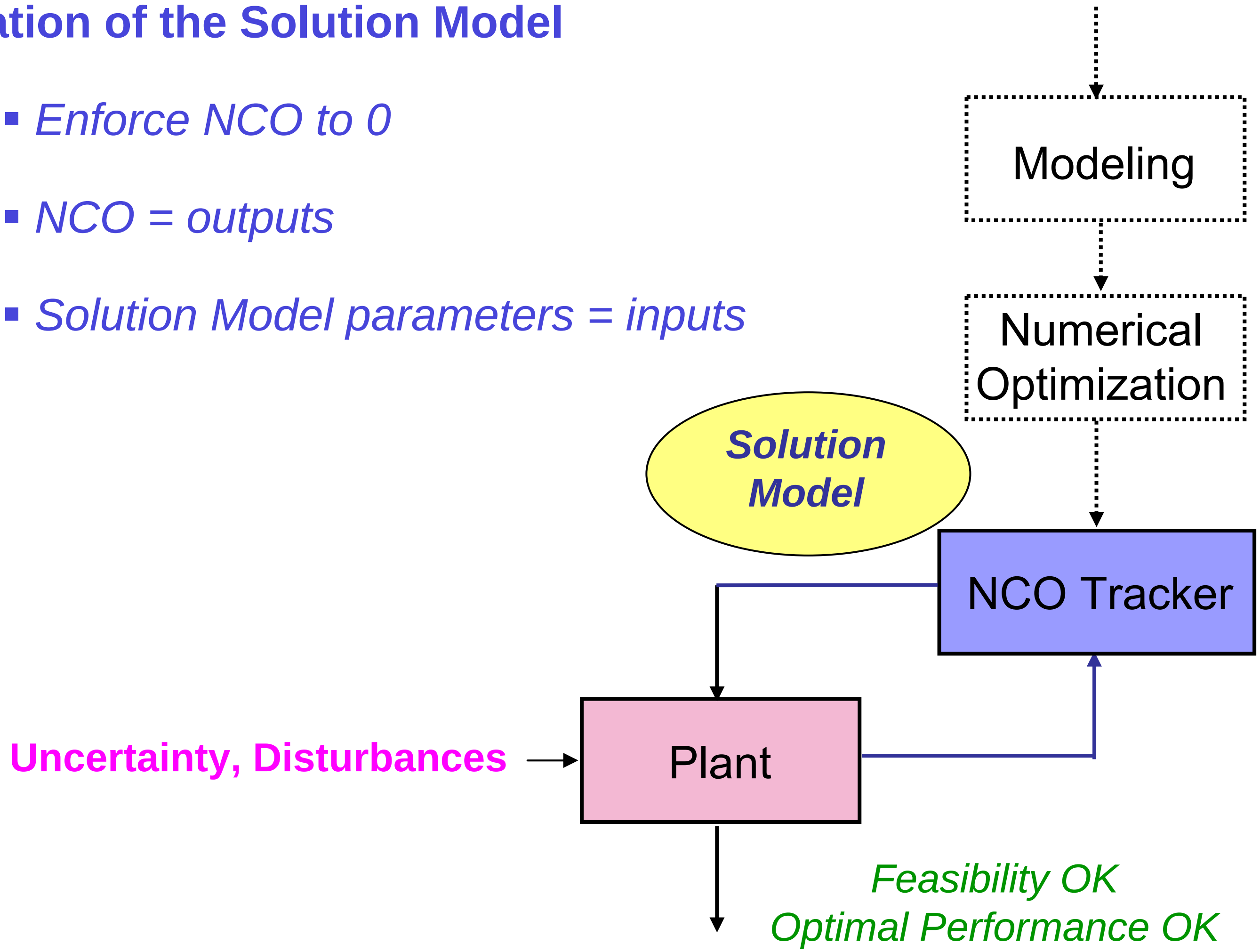
- Control Problem:
  - Inputs, Outputs and Setpoints defined
  - Setpoints uncertainty insensitive
- Optimization Problem:
  - Optimal value (setpoint?) unknown and varies with uncertainty
  - Inputs, Outputs and Setpoints to be defined

**Challenge in MBO**: defining the inputs, the outputs, the setpoints, the control laws that will lead to optimality using appropriate measurements

# Measurement-Based Optimization via NCO-tracking

**Adaptation of the Solution Model**

- *Enforce NCO to 0*
- *NCO = outputs*
- *Solution Model parameters = inputs*



# Model of the Solution

## Input representation with an optimality viewpoint

### Input dissection

Identifies input parts that vary with uncertainty

- Dissect inputs into arcs, use approximations if required
- Identify potential variations of input values with uncertainty

### Assign variables

Links necessary conditions of optimality with input variables

- Identify active path and terminal constraints
- Link free input variables with active constraints

# Necessary Conditions of Optimality

MBO via NCO tracking:

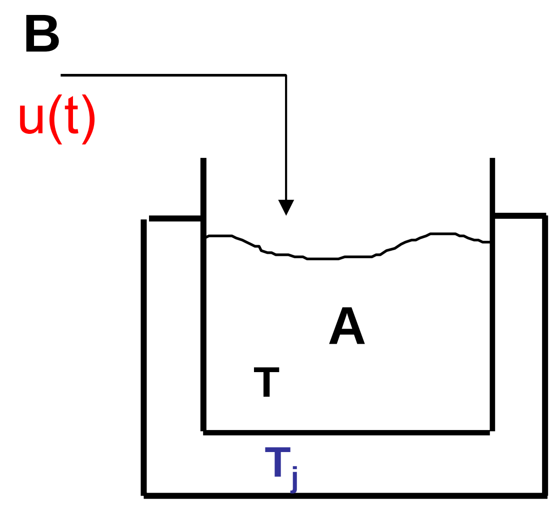
1. NCO from Pontryagin's maximum principle
2. Satisfy 4 objectives in entirely different ways

| | Constraints | Sensitivities |
|---|---|---|
| Path objectives<br>on-line | $S(x, \theta, u) = 0$ | $\partial H / \partial u = 0$<br>H: Hamiltonian |
| Terminal Objectives<br>Off-line | $T(x(\theta, t_f)) = 0$ | $H(t_f) + \left.\frac{\partial \phi}{\partial \pi}\right\|_{t_f} = 0$ |

# Illustrative Example

## Illustrative Example -- Semi-batch Reactor

$$A + B \xrightarrow{k_1} C$$
$$2B \xrightarrow{k_2} D$$




Exothermic reactions -- Isothermal

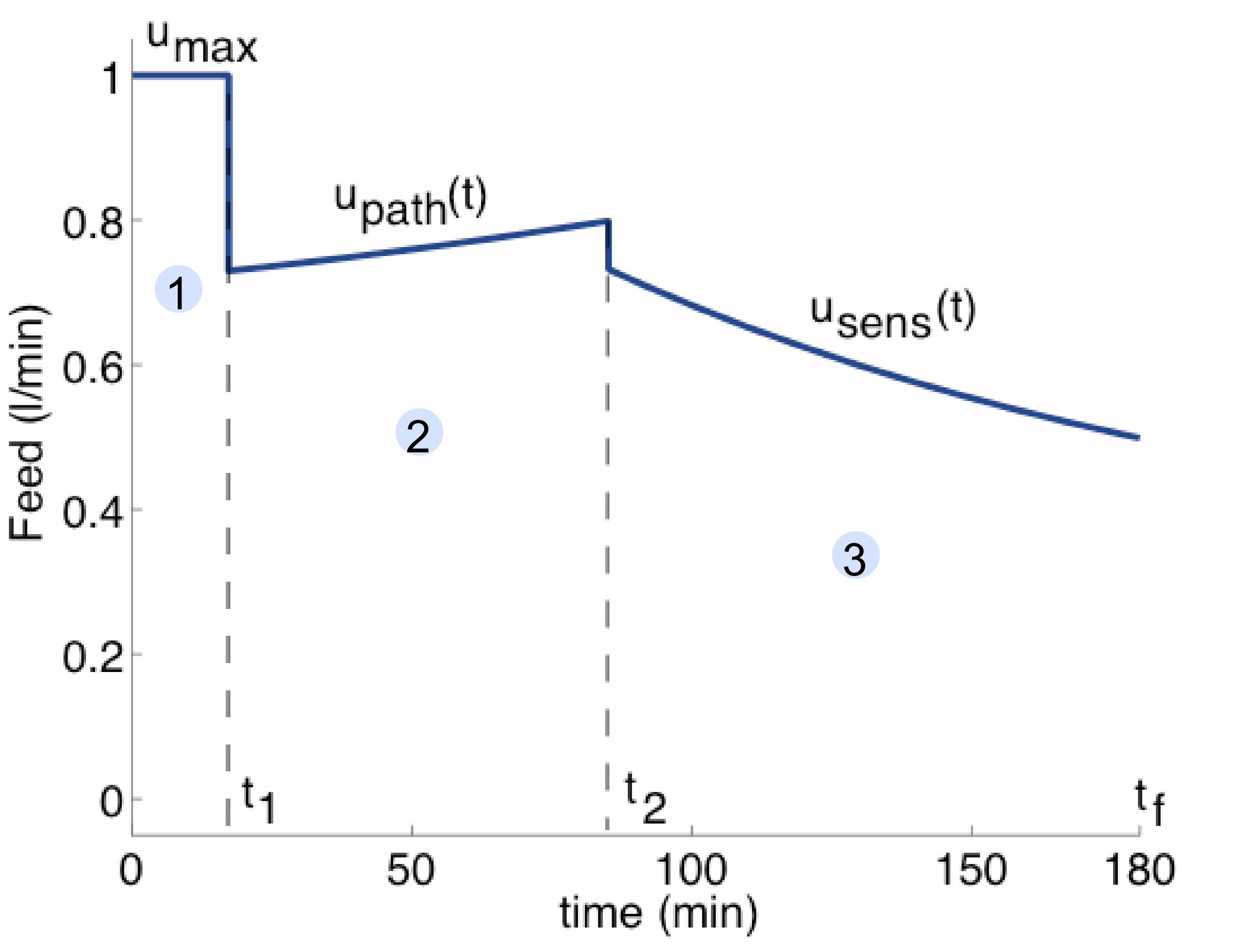
Objective: Maximize number of moles of C at $t_f$ by adjusting u(t)

Safety path constraint: Heat removal limitation $T_j \geq T_{j,min}$

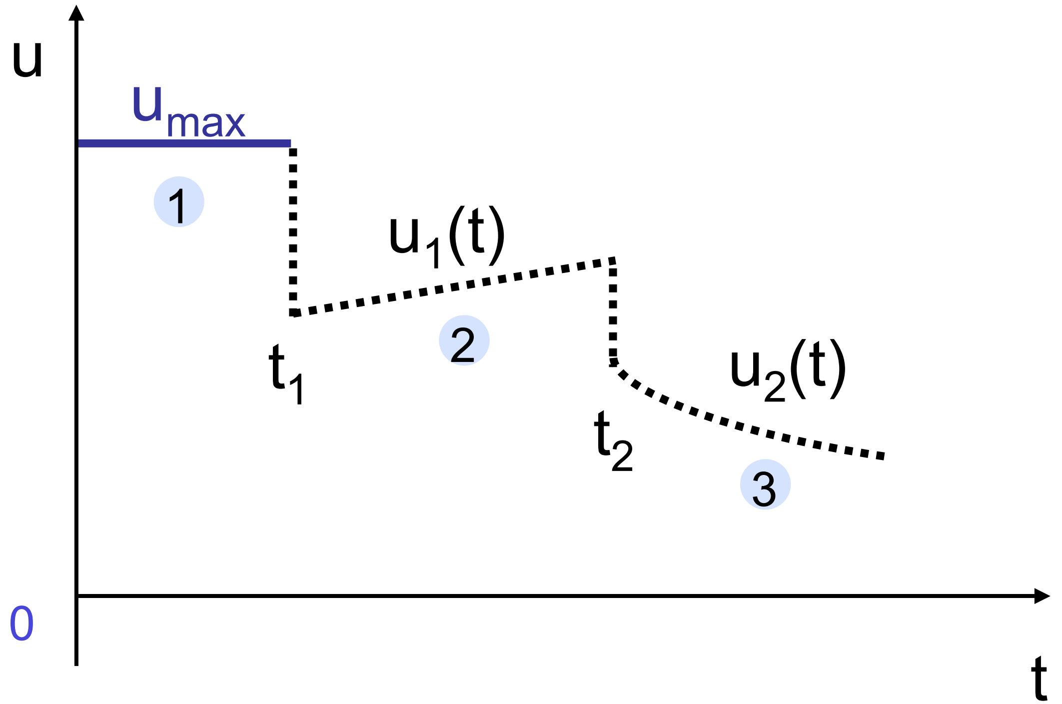
Selectivity terminal constraint: $n_{Df} \leq n_{Df,max}$

# Example of a Model of the Solution

## Nominal Optimal Solution



# Input Dissection




Model → Known (fixed) part -- $u_{max}$

Model → Unknown (free) part -- $t_1$, $t_2$, $u_1(t)$, $u_2(t)$

# Expression of the NCO

**Necessary Conditions of Optimality**
***From Pontryagin's Minimum Principle***

| | Constraints | Sensitivities |
|---|---|---|
| Path Objectives<br>During the run | 2 $T_j = T_{j,min}$ | 3 $\partial H / \partial u = 0$<br>H: Hamiltonian |
| Terminal Objectives<br>End of the run | $n_D(t_f) = n_{Df,max}$ | - |

# Example of a Model of the Solution

## A Solution Model

**Structure Fixed -- no change -- $u_{max}$**

**Adaptation to meet -> path constraints, $T_j = T_{j,min}$ : $t_1$, $u_1(t)$**

**Adaptation to meet -> terminal constraints, $n_D(t_f) = n_{Df,max}$: $t_2$**

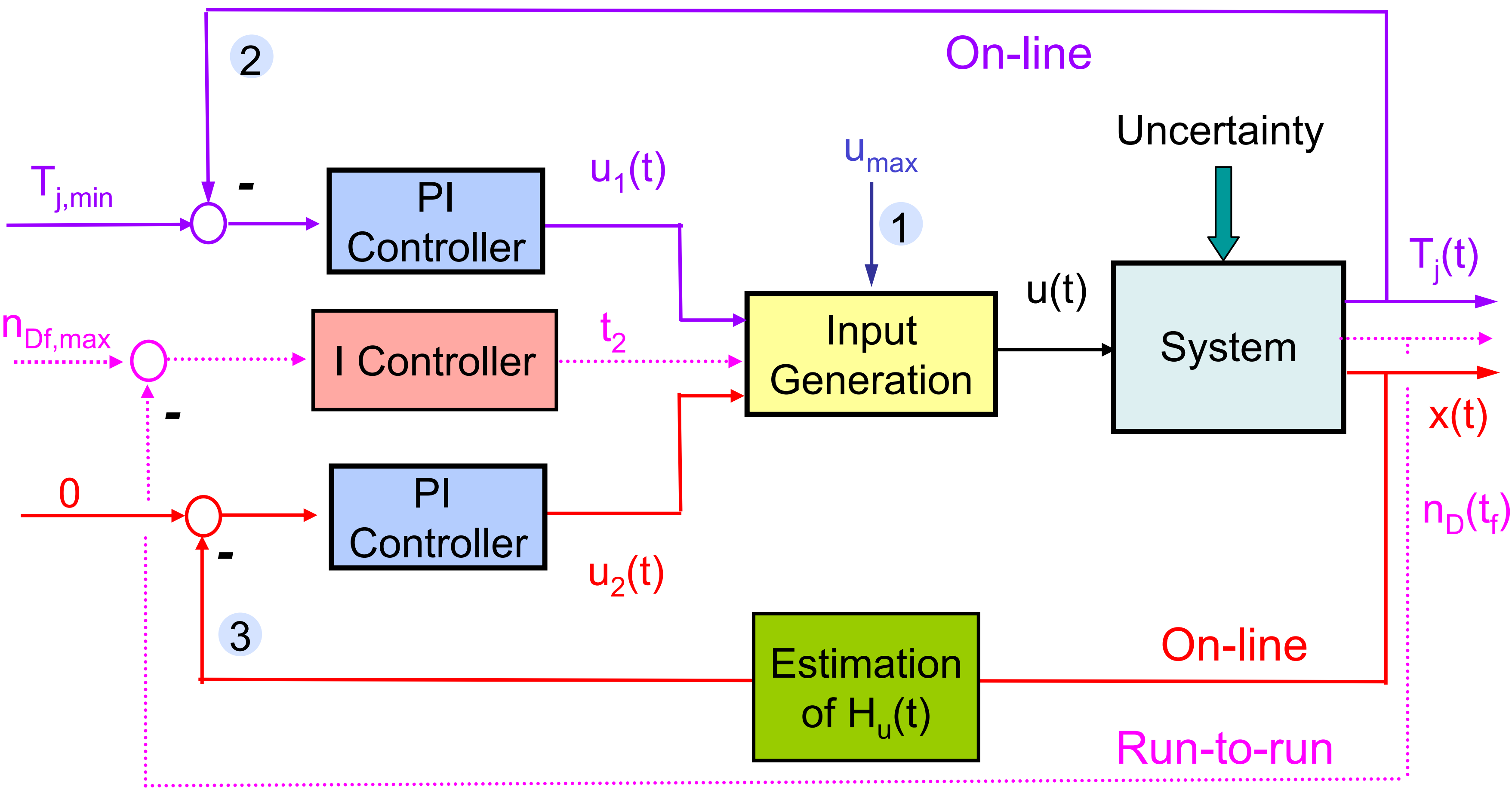
**Adaptation to meet -> sensitivities, $\partial H / \partial u = 0$: $u_2(t)$**

$$u = \begin{cases} u_{max} & 0 \le t \le t_1 \\ u_1 = K_\eta (T_{j,min} - T_j) & t_1 < t \le t_2 \\ u_2 = G_\eta (\partial H / \partial u) & t_2 < t \le t_f \end{cases}$$

$$t_1 = t \quad with \quad T_j(t) = T_{j,min} \quad and \quad T_j(t\_) > T_{j,min}$$

$$t_2 = R_\pi (n_{Df,max} - n_D(t_f))$$

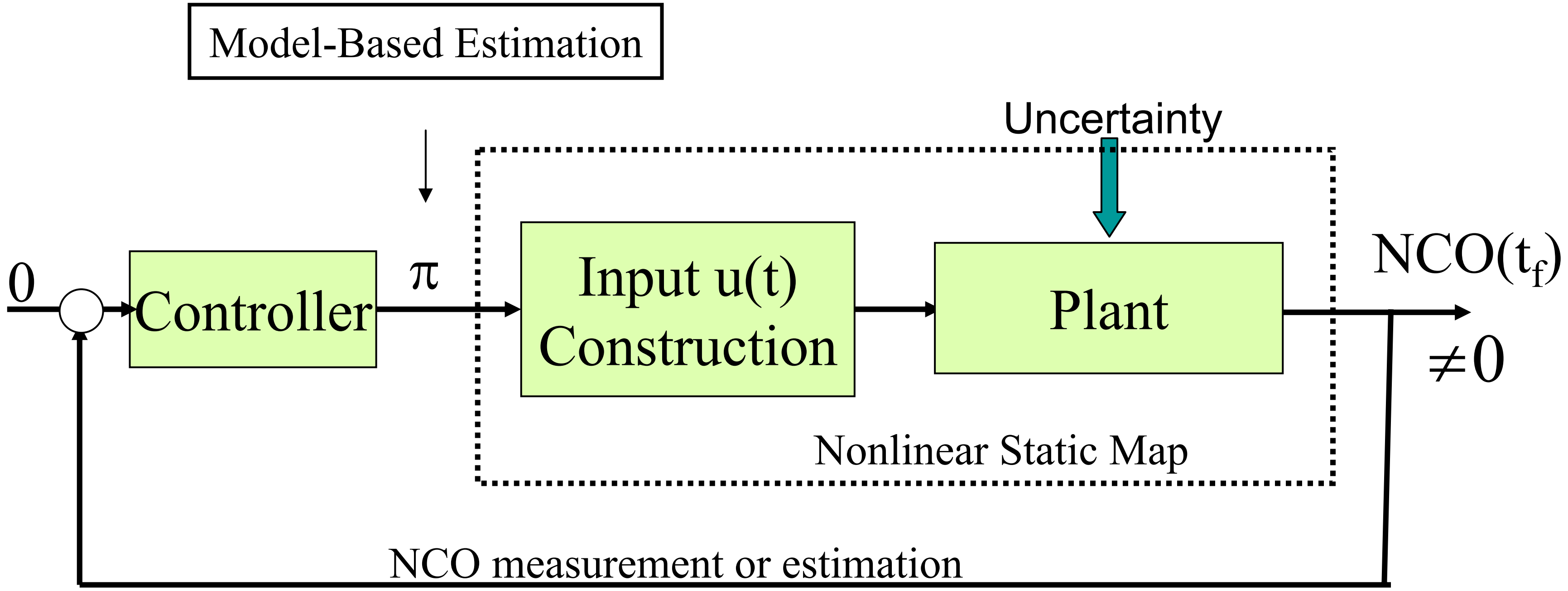
# Example of NCO-tracking Scheme



# Outline

- Background
- Dynamic Optimization of Batch Processes
- Measurement-Based Optimization
  - Choice of Manipulated Variables: Solution Model
  - Tracking the Necessary Conditions of Optimality
- Run-to-Run optimization:
  - Influence of Uncertainty and Input Decoupling
  - Controller Structure and Convergence Analysis
- Application to Industrial Acrylamide Copolymerization
- Conclusion & Perspectives

# Measurement-Based Run-to-Run Optimization




Run-to-Run Optimization <-> Static Optimization

# Static Optimization Formulation

- Assumptions:
  - Set of Active Constraints does not vary with uncertainty
  - Remove inactive constraints
  - Equality Constraints
  - More parameters than constraints ($n_\pi \geq \tau$)
- Problems:
  - NCO coupled
  - Lagrange multipliers unknown
  - Need for $\pi$ decoupling
  - $n_\pi + \tau$ equations for determining $n_\pi$ parameters

$$\min_{\pi}\left(\phi\left(\theta,\pi\right)\right)$$

$$s.t.: T\left(\theta,\pi\right)=0$$

$$NCO:$$

$$\begin{cases} \upsilon^T T(\theta,\pi) = 0 \\ \dfrac{\partial\phi(\theta,\pi)}{\partial\pi} + \upsilon(\theta)^T \dfrac{\partial T(\theta,\pi)}{\partial\pi} = 0 \end{cases}$$

# Input Separation

Separate parameters depending on their effect on Constraints

- Gain Matrix G = dT/dπ (model, or experiments)
- SVD of G separates constraint and sensitivity-seeking parameters (second level of separation possible)

$$T(\theta, \bar{\pi}, \tilde{\pi}) = 0 \quad \longrightarrow \quad \textit{provides } \bar{\pi}, \tau \textit{ eq.}$$

$$\left(\frac{\partial \phi}{\partial \bar{\pi}}\right)^T + \left(\frac{\partial T}{\partial \bar{\pi}}\right) \nu = 0 \quad \longrightarrow \quad \textit{allows computing } \nu$$

$$\left(\frac{\partial \phi}{\partial \tilde{\pi}}\right)^T = 0 \quad \longrightarrow \quad \textit{provides } \tilde{\pi}, (n_\pi - \tau) \textit{ eq.}$$

# Input Separation: Expression of the Variation of the NCO

$$\Delta T = \frac{\partial T}{\partial \bar{\pi}} \Delta \bar{\pi} + \frac{\partial T}{\partial \theta} \Delta \theta$$

$$\Delta \left( \frac{\partial \phi}{\partial \tilde{\pi}} \right)^T = \left( \frac{\partial^2 \phi}{\partial \tilde{\pi}^2} \right) \Delta \tilde{\pi} + \left( \frac{\partial^2 \phi}{\partial \bar{\pi} \partial \tilde{\pi}} \right) \Delta \bar{\pi} + \left( \frac{\partial^2 \phi}{\partial \theta \partial \tilde{\pi}} \right) \Delta \theta$$

- More Simple Expression
- Defines the Control Laws for Constraint-Seeking and Sensitivity - Seeking Parameters, with respect to measurements of the deviation of the NCO

$$\Delta \bar{\pi} = -\left( \frac{\partial T}{\partial \bar{\pi}} \right)^{-1} \frac{\partial T}{\partial \theta} \Delta \theta = -\left( \frac{\partial T}{\partial \bar{\pi}} \right)^{-1} T_m$$

$$\Delta \tilde{\pi} = -\left( \frac{\partial^2 \phi}{\partial \tilde{\pi}^2} \right)^{-1} \left[ -\frac{\partial^2 \phi}{\partial \bar{\pi} \partial \tilde{\pi}} \left( \frac{\partial T}{\partial \bar{\pi}} \right)^{-1} \frac{\partial T}{\partial \theta} + \frac{\partial^2 \phi}{\partial \theta \partial \tilde{\pi}} \right] \Delta \theta = -\left( \frac{\partial^2 \phi}{\partial \tilde{\pi}^2} \right)^{-1} \left( \frac{\partial \phi}{\partial \tilde{\pi}} \right)_m^T$$

# From Control Laws to Integral Run-to-Run Update

$$\Delta\bar{\pi} = -\left(\frac{\partial T}{\partial\bar{\pi}}\right)^{-1}\frac{\partial T}{\partial\theta}\Delta\theta = -\left(\frac{\partial T}{\partial\bar{\pi}}\right)^{-1}T_m$$

$$\Delta\tilde{\pi} = -\left(\frac{\partial^2\phi}{\partial\tilde{\pi}^2}\right)^{-1}\left[-\frac{\partial^2\phi}{\partial\bar{\pi}\partial\tilde{\pi}}\left(\frac{\partial T}{\partial\bar{\pi}}\right)^{-1}\frac{\partial T}{\partial\theta}+\frac{\partial^2\phi}{\partial\theta\partial\tilde{\pi}}\right]\Delta\theta = -\left(\frac{\partial^2\phi}{\partial\tilde{\pi}^2}\right)^{-1}\left(\frac{\partial\phi}{\partial\tilde{\pi}}\right)_m^T$$

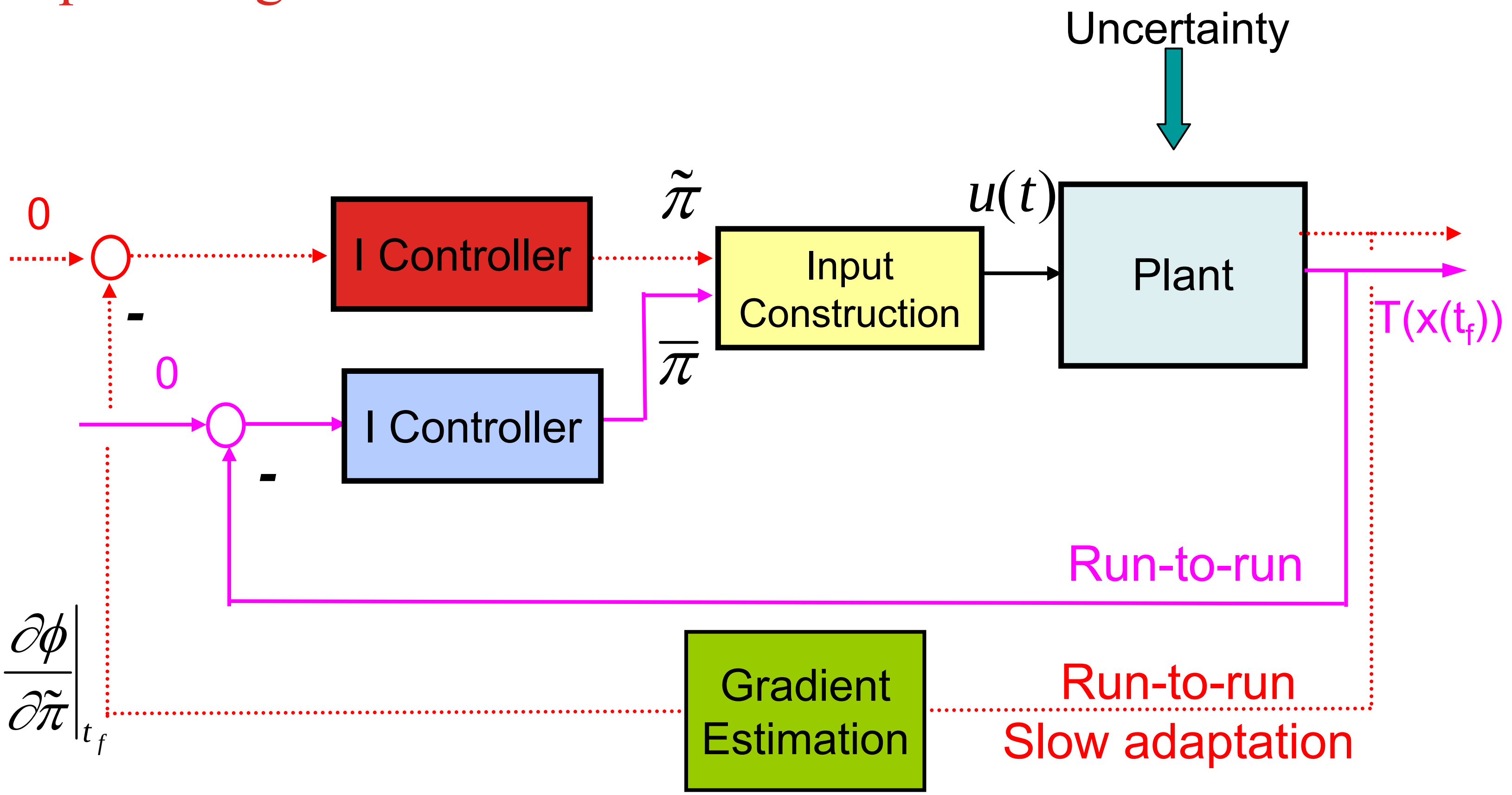
$$\bar{\pi}(k+1) = \bar{\pi}(k) - K_1\hat{\bar{G}}^{-1}T_m(k)$$

$$\tilde{\pi}(k+1) = \tilde{\pi}(k) - K_2\hat{\tilde{H}}^{-1}\left(\frac{\partial\phi}{\partial\tilde{\pi}}\right)_m^T(k)$$

- Uses fixed estimates of gain and Hessian matrices (invertible)
- Only equilibrium point that corresponds to NCO = 0

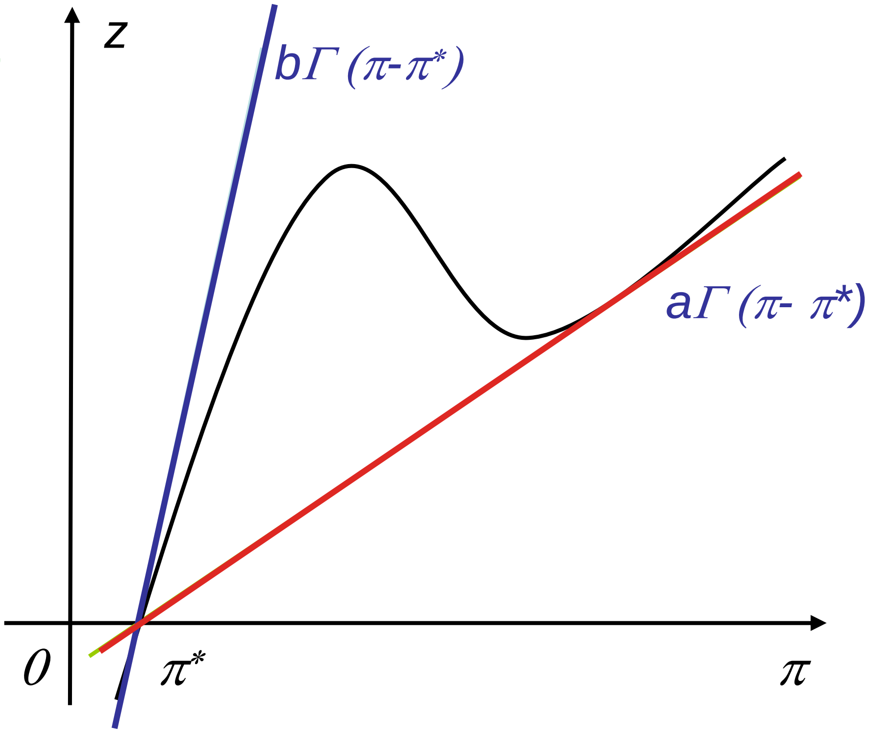
# Run-to-Run Control Scheme

## Example: Integral Run-to-run

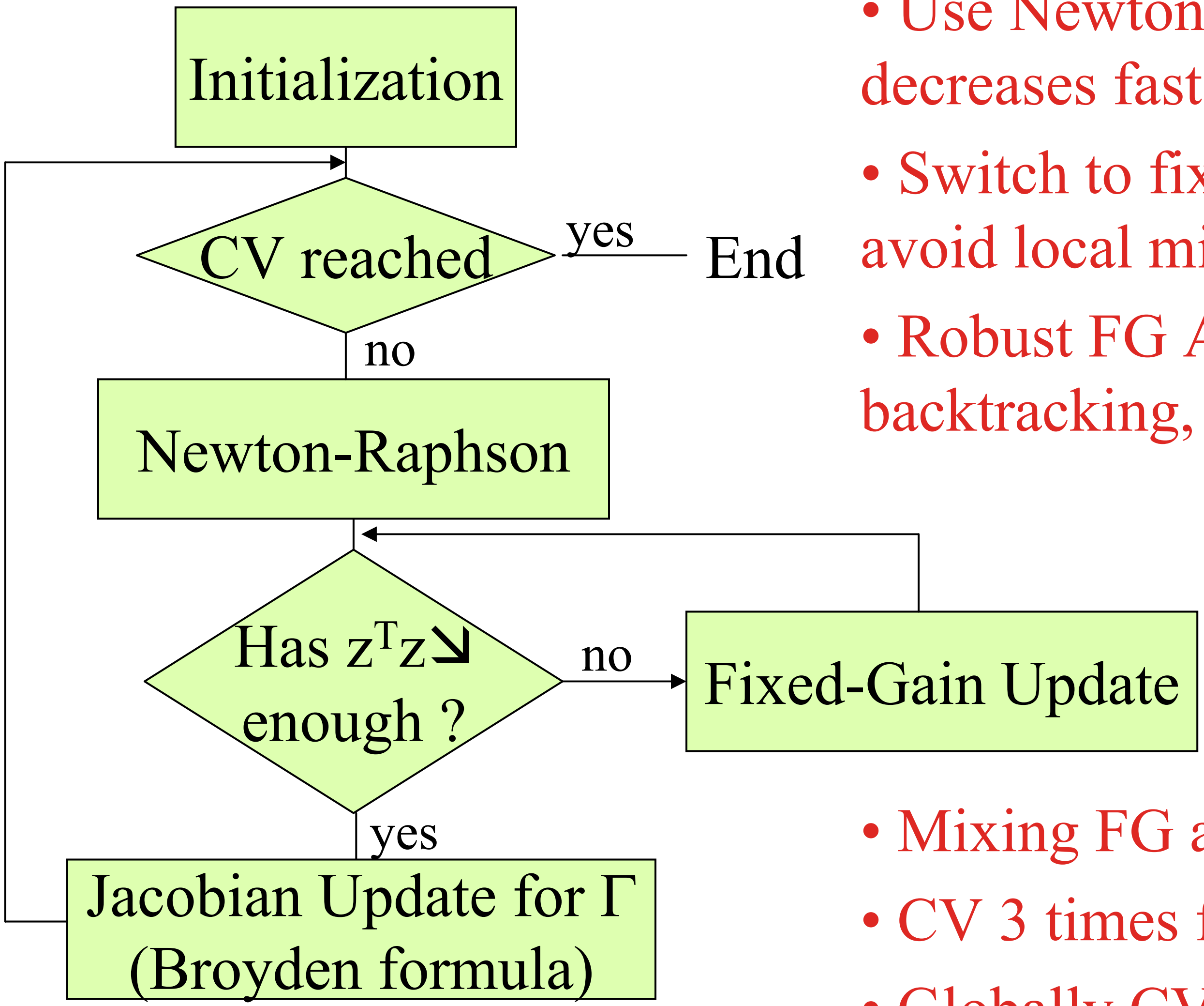


# Convergence Analysis of the 2 closed-loops

- Global MIMO Convergence
- Sector nonlinearities
  - $(z - a\Gamma(\pi-\pi^*))^T(b\Gamma(\pi-\pi^*) - z) > 0$
  - $\Gamma$ = estimate of gain or Hessian
  - $(\pi_k-\pi^*)\ \Gamma^T\Gamma(\pi_k-\pi^*)$ is Lyapunov
  - Provides limit values for K
  - Fixed-Gain
- R2R = Solving Sets of Nonlinear equations $z(\pi) = 0$
  - Fixed-Gain can be slow
  - Second Algorithm to speed up CV
  - test function $z^Tz$



# Convergence Analysis (2)




- Use Newton-Raphson when $z^Tz$ decreases fast enough
- Switch to fixed algorithm to avoid local minima
- Robust FG Algo. replaces backtracking, and / or line search

- Mixing FG and Variable Gain
- CV 3 times faster
- Globally CV

# Outline

- Background
- Dynamic Optimization of Batch Processes
- Measurement-Based Optimization
  - Choice of Manipulated Variables: Solution Model
  - Tracking the Necessary Conditions of Optimality
- Run-to-Run optimization:
  - Influence of Uncertainty and Input Decoupling
  - Controller Structure and Convergence Analysis
- Application to Industrial Acrylamide Copolymerization
- Conclusion & Perspectives

# Application to Industrial Acrylamide Copolymerization

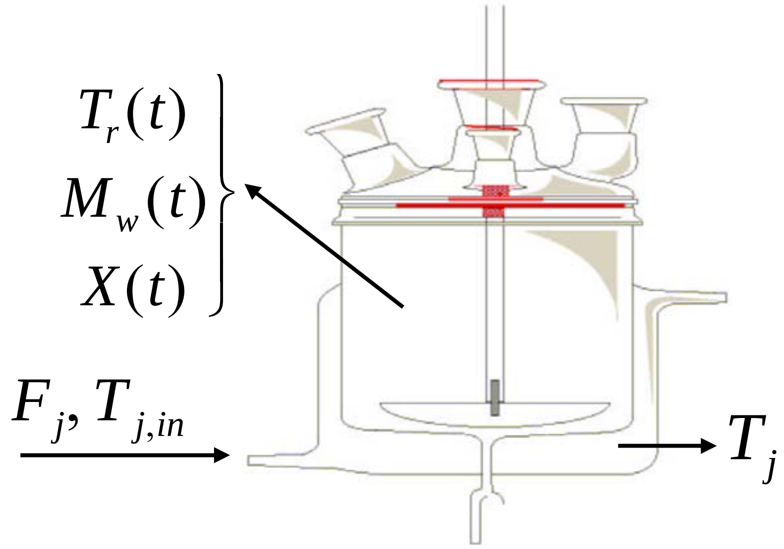
AQUA+TECH SPECIALTIES SA

- Inverse-emulsion copolymerization of acrylamide with quaternary ammonium cationic monomer(s)
  - Copolymer used as flocculant for wastewater treatment
  - Monomers -- toxic, copolymer -- edible $\Rightarrow$ >99.99% conversion

- Organic-phase reactions
  - Initiator decomposition
  - Propagation
  - Reactions of primary radicals
  - Transfer between phases

- Aqueous-phase reactions
  - Propagation
  - Reactions of primary radicals
  - Addition to terminal double bounds
  - Transfer to monomer
  - Termination with emulsifier
  - Termination by disproportionation

# Application to Industrial Acrylamide Copolymerization




Input Bound: $T_r(t) \leq T_{r,max}$

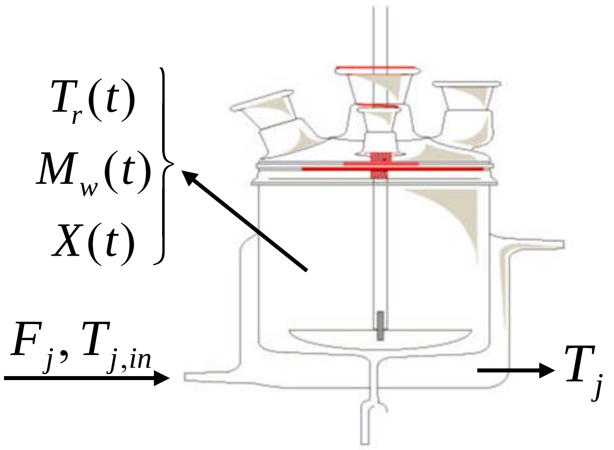
Path Constraint: $T_{j,in}(t) \geq T_{j,in,min}$

Terminal Constraints: $\begin{cases} M_w(t_f) \geq M_{w,des} \\ X(t_f) \geq X_{des} \end{cases}$

# Application to Industrial Acrylamide Copolymerization

AQUA+TECH SPECIALTIES SA

- Industrial features
  - 1, 3, 8-ton reactors, risk of runaway
  - Initiator efficiency can vary considerably
  - Several recipes
    - different initial conditions
    - different initiator feeding policies
    - use of chain transfer agent
    - use of cross-linking/branching agent




- Modeling difficulties
- Uncertainty

- Challenge: Implement (near) optimal operation for various recipes

# Application to Industrial Acrylamide Copolymerization

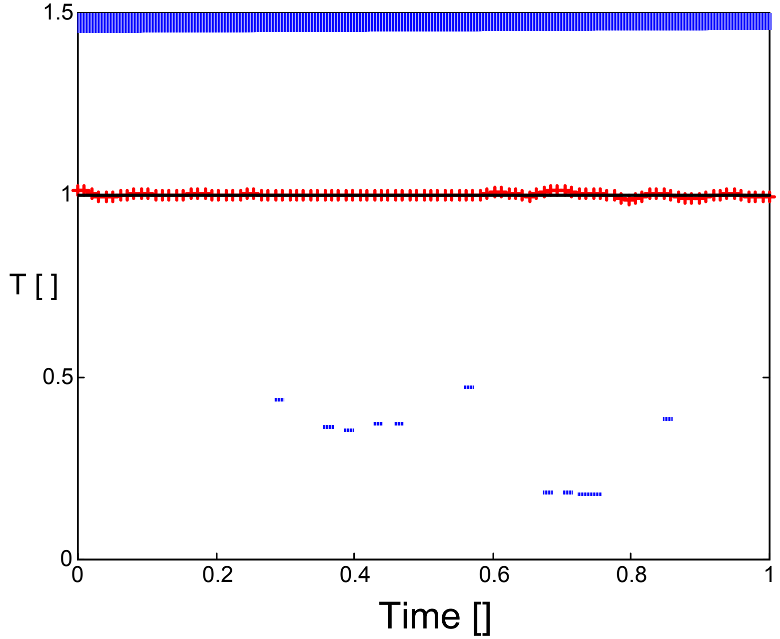
AQUA+TECH SPECIALTIES SA

- Tendency Model
  - 7 Differential equations + Algebraic Equations
  - Precise Enough to Describe the Main Phenomena
  - Good Estimation of the Conversion Profile
  - Moments Distribution for the Computation of the Molecular Weight Distribution
  - Terminology of Homopolymerization
  - Parameters tuned to match industrial Reality

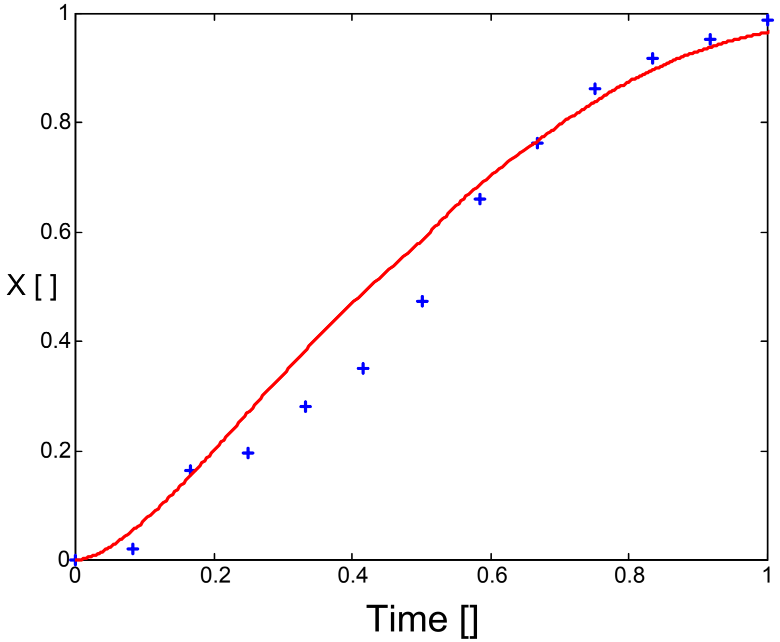
# Application to Industrial Acrylamide Copolymerization

## Industrial Practice

### From Initiation to 98.5% Conversion




- Temperature setpoint
+ Reactor temperature
- Jacket temperature

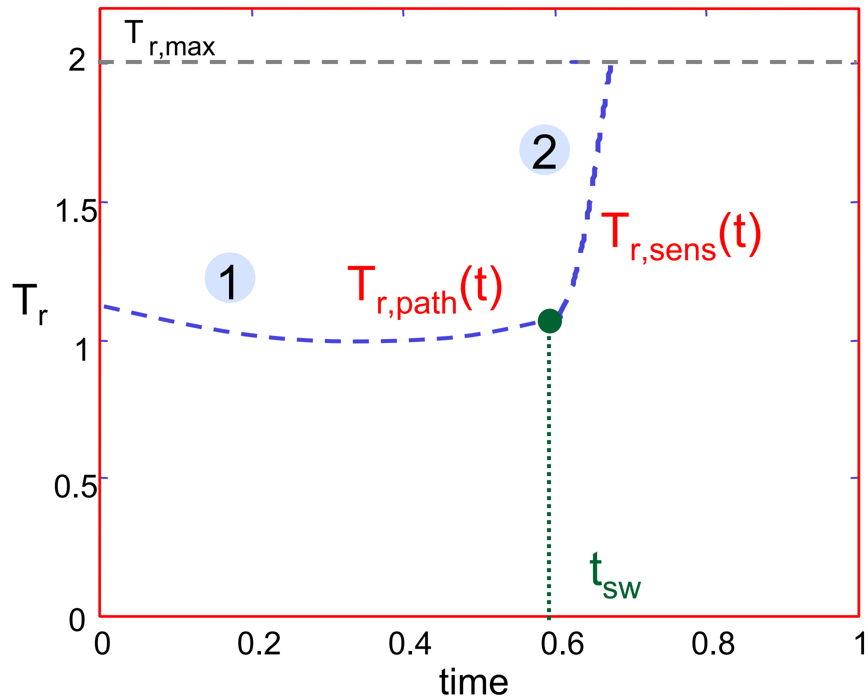



+ Conversion measurements
- Predicted conversion (tendency model)

# Application to Industrial Acrylamide Copolymerization

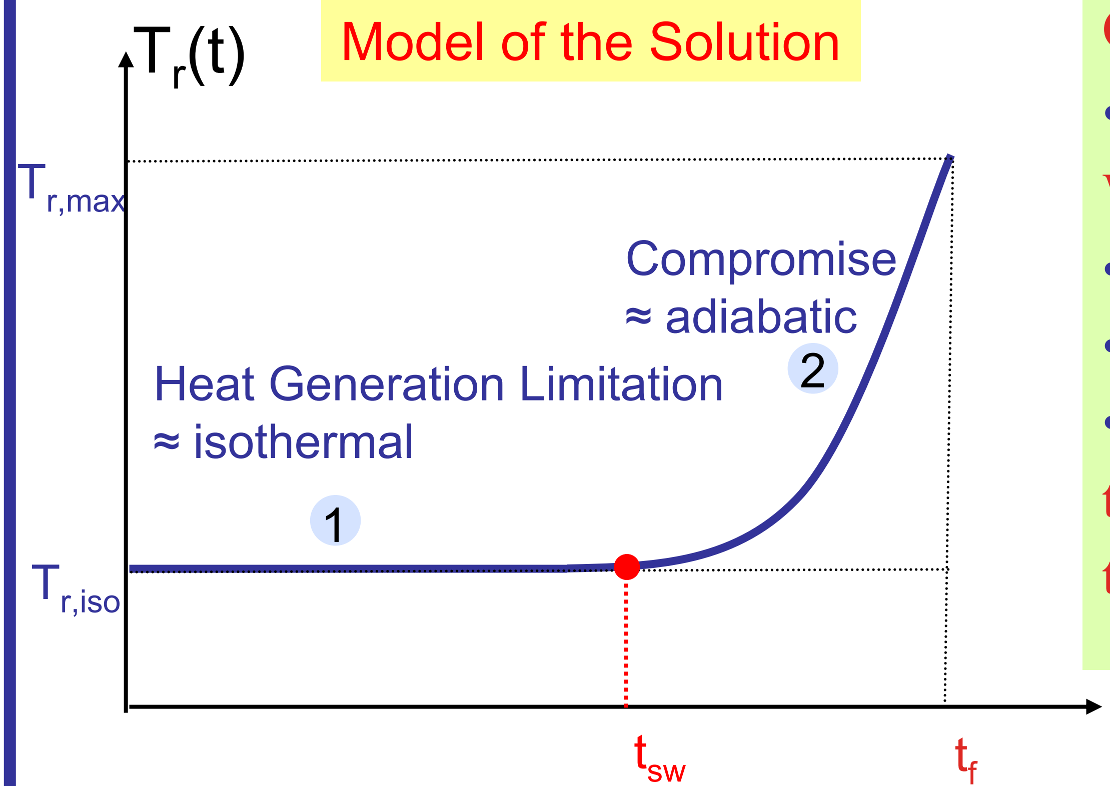
AQUA+TECH SPECIALTIES SA

## Nominal Optimization




- Arc 1: Heat removal constraint
- Arc 2: Compromise between conversion and molecular weight
- Switching time: To meet molecular weight terminal constraint

# Model of the Solution: Semiadiabatic Profile




Compromise:

- ⬀ T, ⬀ X, ⬂ $M_w$:

With SA

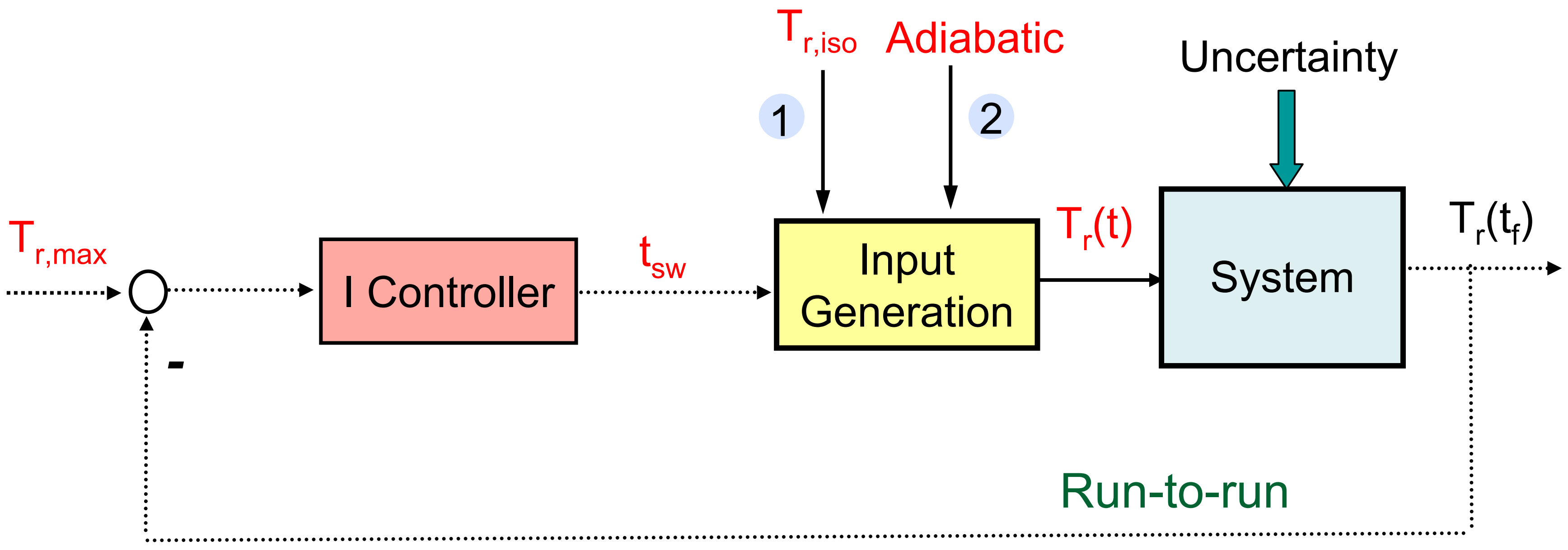
- Constraints OK
- Trade-Off OK
- Structure Fixed

$t_{sw}$, $t_f$ + Structure ⇨ u(t)

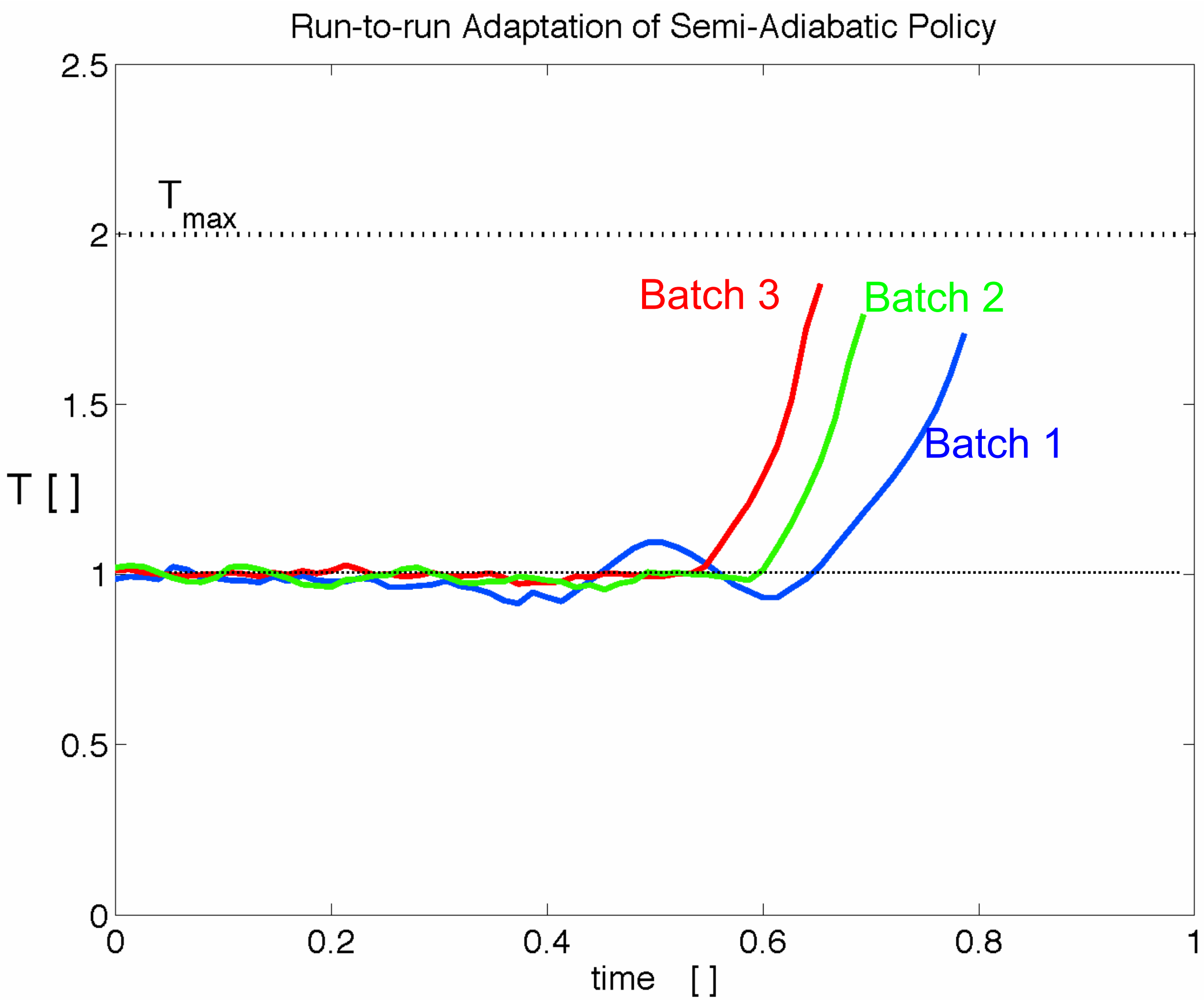
$t_f$ defined upon reaching $X_{des}$

- $T_{r,max}$ + restrictive than $M_{w,des}$
- $t_{sw}$ adapted to meet $T_{r,max}$

# Run-to-Run Scheme



# Results




Final Time

- Isothermal: 1.00
- Batch 1: 0.78
- Batch 2: 0.72
- Batch 3: 0.65

# Conclusions & Perspectives

- Methodology
  - Variations of Path Objectives
  - Quantify the quality of the solution model
  - On-line corrections to satisfy terminal objectives (trajectory following)
  - Local Vs Global ??
  - What happens if the set of active constraints changes (MPC …)
- Run-to-Run Optimization
  - Extend the class of systems
  - Include other kinds of objectives (economical, …)
- What about the rest of the plant ?
  - Interest of being optimal at the scale of 1 reactor ?
  - Divide a large scale problem into pieces -> MBO
  - Control at the scale of the plant using a “super structure”

END

# Conclusions & Perspectives

- Methodology
  - define an typical optimal profile for anaerobic digester start-up
  - parameterize the input
  - control to force CNO = 0

- First study on extended AM2 model for fixed-bed A.D.
  - without constraint $S_{in}$, $Q_{in}$ go to their upper bounds = substrate inhibition might be neglected
  - if constraint on depollution rate = dominant
    - *assign $Q_{in}$ to control substrate conversion to its lower limit*
  - $H_2$ inhibits cells growing
    - *assign $S_{in}$ to control $H_2$ to a low value*

# Bibliography

## Journal Articles:


1. François G., Srinivasan, B. & Bonvin D.,"*Use of Measurements for Enforcing the Necessary Conditons of Optimality in the Presence of Constraints and Uncertainty*", **Journal of Process Control**, Vol. 15, pages 701-712, 2005
2. François G., Srinivasan, B. & Bonvin D., "*Run-to-run Adaptation of a Semiadiabatic Policy for the Optimization of an Industrial Batch Polymerization Process*", **I&ECR**, Vol. 43, N. 23, pages 7238-7243, 2004
3. Lima R., François G., Srinivasan B. & R.Salcedo,"*Dynamic Optimization of Batch Emulsion Polymerization using MSIMPSA, a Simulated-Annealing-Based Algorithm*", **I&ECR**, Vol 43, N. 24, pages 7796-7806, 2004
4. Srinivasan B., D. Bonvin, E. Visser and S. Palanki. "*Dynamic Optimization of Batch Processes: II. Role of Measurements in Handling Uncertainty*". **Comput. Chem. Engng**., 2003, 27, 27-44
5. Srinivasan B., S. Palanki and D. Bonvin. "*Dynamic Optimization of Batch Processes: I. Characterization of the Nominal Solution*". **Comput. Chem. Engng**., 2003, 27, 1-26

# Bibliography (2)

Conference Proceedings:


1. "Run-to-run Optimization of Batch Emulsion Polymerization", IFAC 2002, Barcelone, pages 1258-1263
2. "Convergence Analysis of a Run-to-Run Control for a Class of Nonlinear Systems", ACC 2003, Denver, pages 3032-3037
3. "Trajectory Following for the Optimization of a Batch Polymerization Reactor", BatchPro Symposium PrePrints, Poros (Greece), 2004, pages 135-159
4. "A Globally Convergent Run-to-Run Algorithm with Improved Rate of Convergence", ACC 2005, Portland

# Bibliography (3)

Conference Proceedings:

5. “Measurement-Based Optimization of an Emulsion Polymerization Process”, Polymer Reaction Engineering: Modeling, Optimization and Control, Lyon, 2003, pages 108-110.

6. “Run-to-Run Optimization of Batch Styrene Copolymerization”, Polymer Reaction Engineering: Modeling, Optimization and Control, Lyon, 2003, pages 16-19.