MODEL-BASED CONTROL OF PARTICULATE PROCESSES

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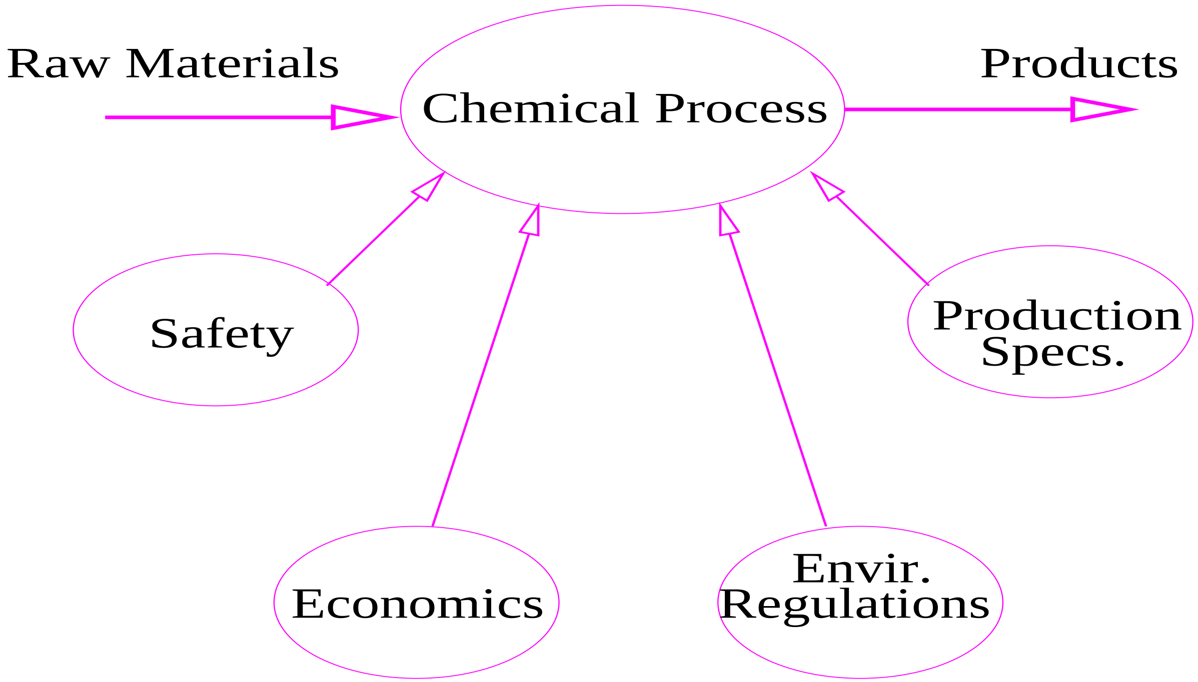
INTRODUCTION

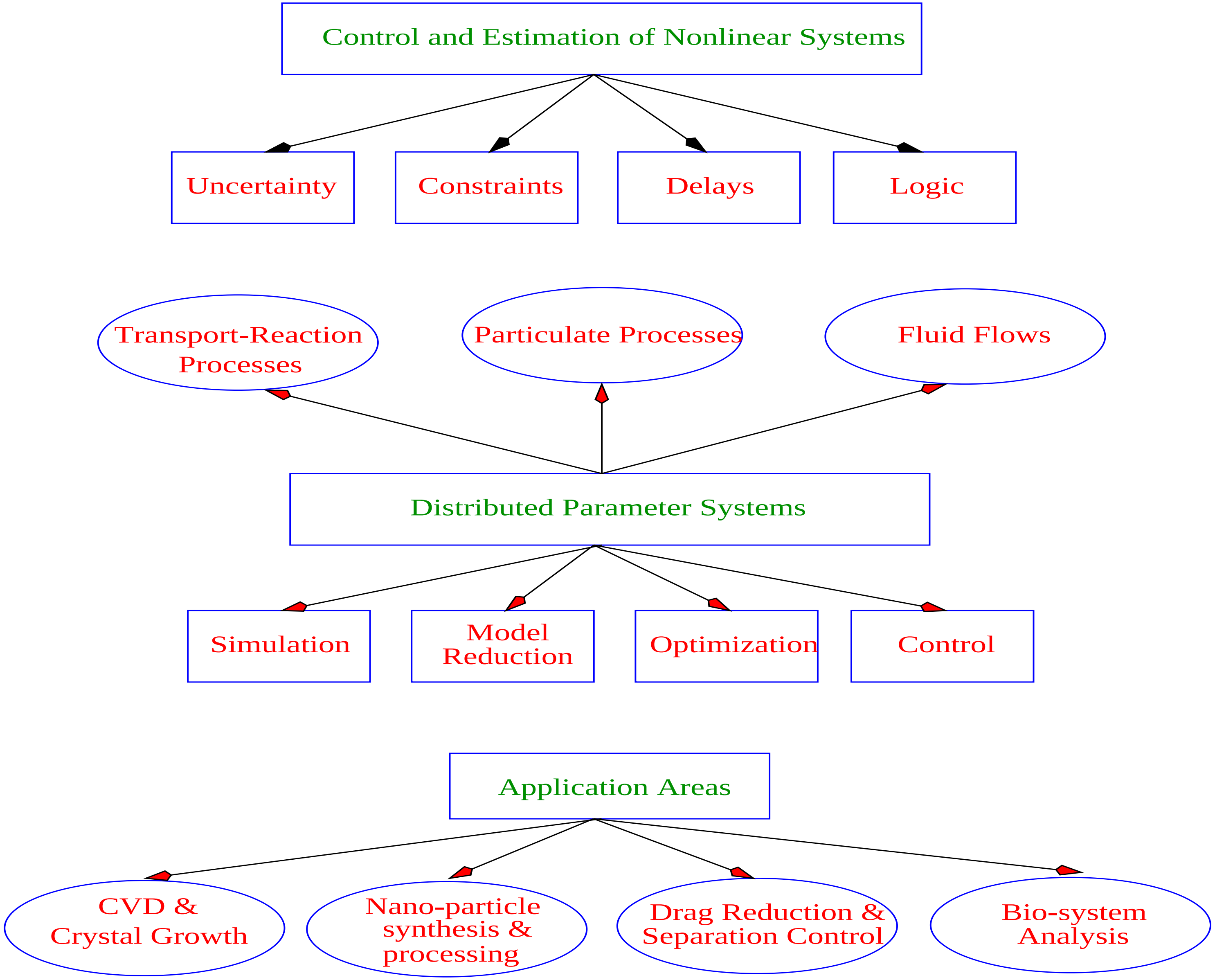
- Incentives for chemical process control.



  ◇ Need for continuous monitoring and external intervention (control).

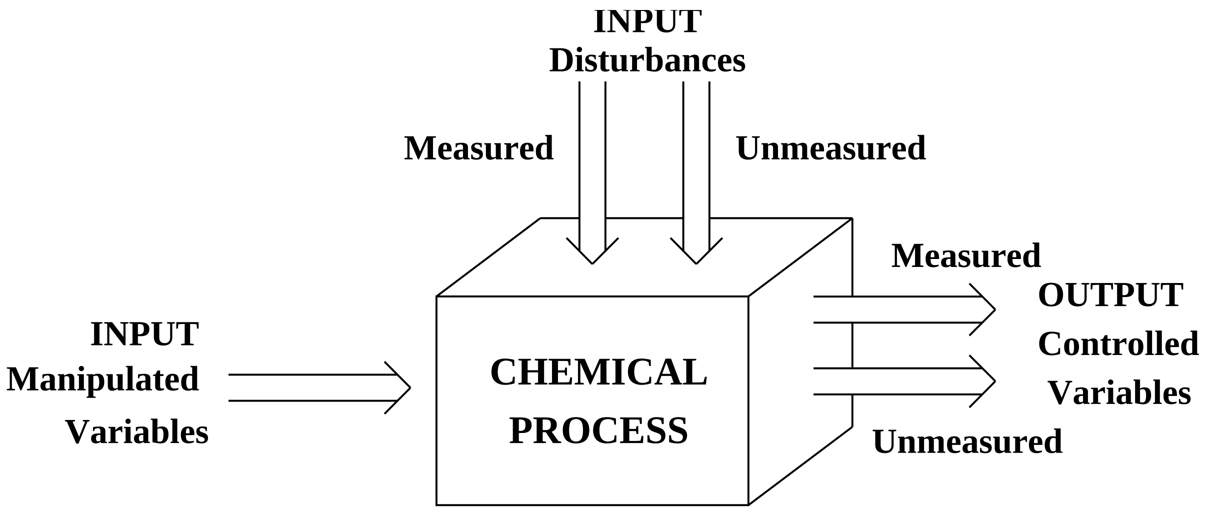
- Objectives of a process control system.
  ◇ Ensuring stability of the process.
  ◇ Suppressing the influence of external disturbances.
  ◇ Optimizing process performance.

PROCESS CONTROL RESEARCH IN OUR GROUP

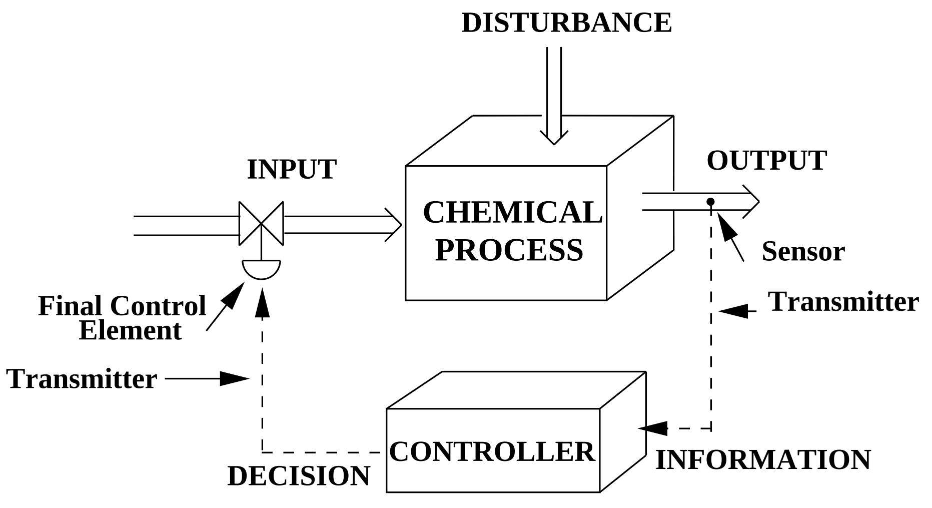


BASIC CONCEPTS IN PROCESS CONTROL

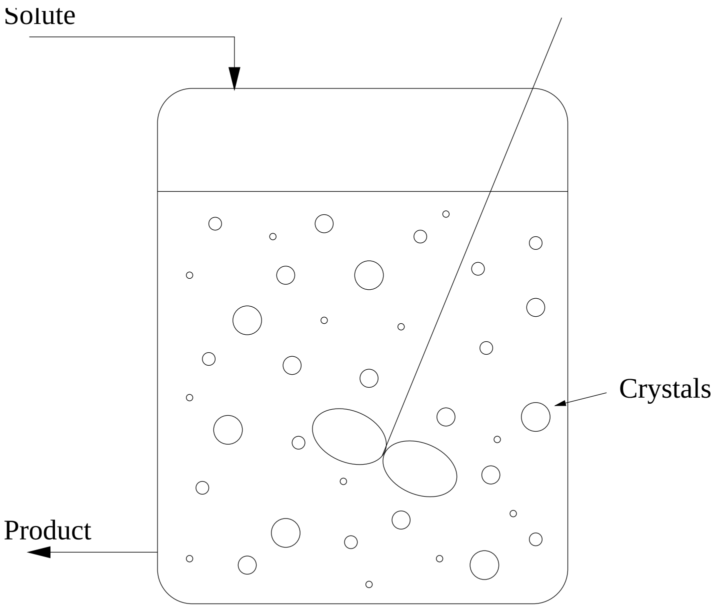
- Process variables.



- Feedback control loop.



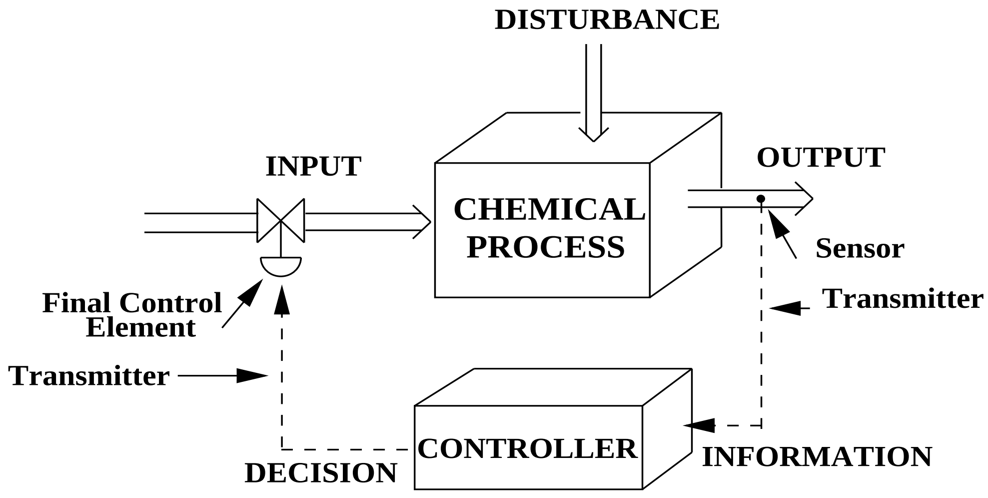
A CONTINUOUS CRYSTALLIZER



- **Manipulated variables**
  - ◇ Solute concentration
  - ◇ Inlet stream flow rate
  - ◇ Seeding
  - ◇ Heating/Cooling
- **Measured output variables**
  - ◇ Crystal concentration
  - ◇ Solute concentration
  - ◇ Crystal size distribution
- **Controlled output variables**
  - ◇ Crystallization stability
  - ◇ Shaping crystal size distribution

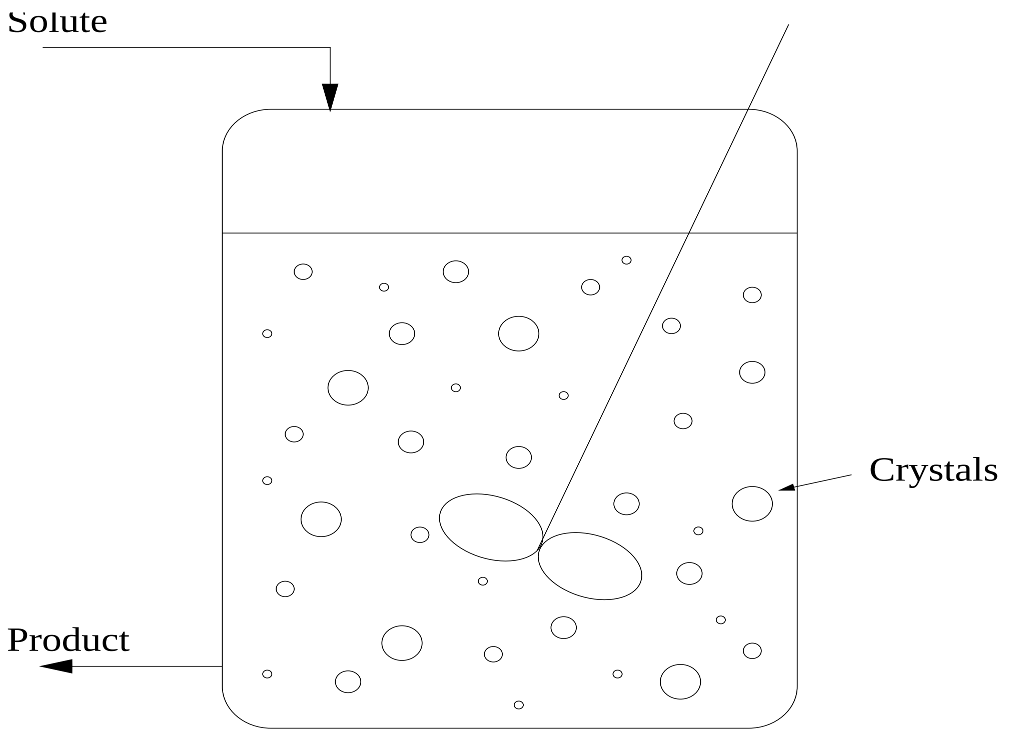
APPROACHES TO CONTROLLER DESIGN

- Feedback control loop.



- Approaches to controller design
  - ◇ Classical control
    - ▷ Proportional control
    - ▷ Proportional-Integral control
    - ▷ Proportional-Integral-Derivative Control
  - ◇ Model-based control
    - ▷ Nonlinear control
    - ▷ Optimization-based control (Model Predictive Control)

A CONTINUOUS CRYSTALLIZER: MODELING



- **Modeling assumptions:**
  - ◇ Perfect mixing and isothermal operation.
  - ◇ No particle breakage and agglomeration.
  - ◇ No product classification.

MATHEMATICAL MODEL

- **Nucleation:**

$$\boxed{Q(t) = \epsilon k_2 exp\left(-\frac{k_3}{\left(\frac{c}{c_s}-1\right)^2}\right)}$$

- **Growth:**

$$\boxed{R(t) = k_1(c - c_s)}$$

- **Population balance equation:**

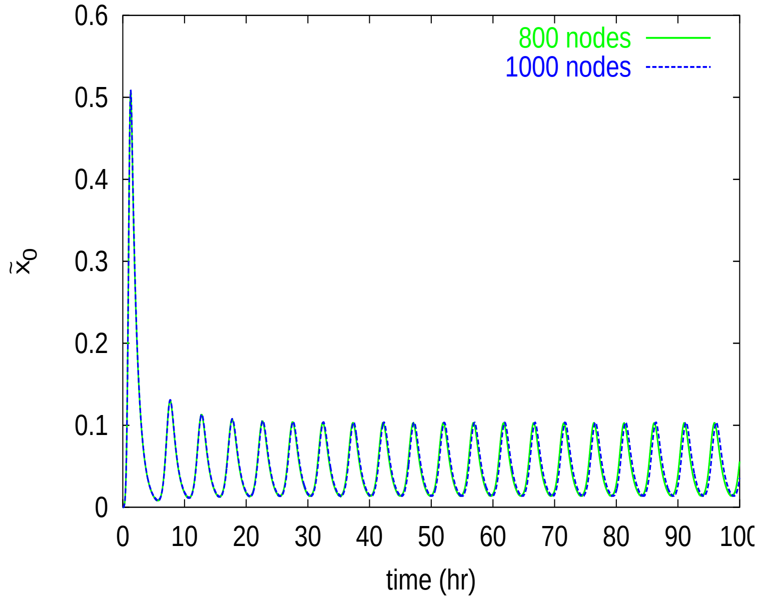
$$\boxed{\frac{\partial n}{\partial t} = -\frac{\partial (R(t)n)}{\partial r} - \frac{n}{\tau}, \quad n(0,t) = Q(t)/R(t)}$$

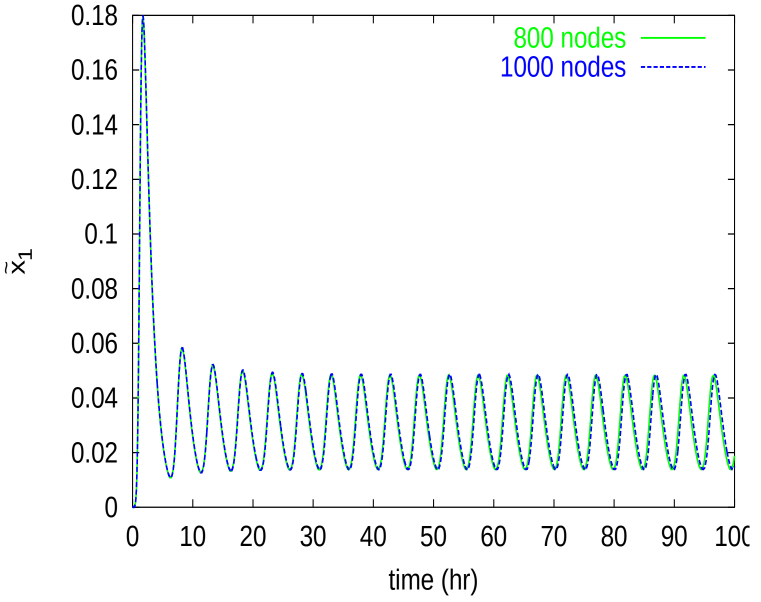
- **Mass balance equation:**

$$\boxed{\begin{aligned} \frac{dc}{dt} &= \frac{(c_0 - \rho)}{\epsilon\tau} + \frac{(\rho - c)}{\tau} + \frac{(\rho - c)}{\epsilon}\frac{d\epsilon}{dt} \\ \epsilon &= 1 - \int_0^\infty n(r,t)\frac{4}{3}\pi r^3 dr \end{aligned}}$$

OPEN-LOOP BEHAVIOR

- Unique unstable steady-state surrounded by limit cycle.
- Open-loop profile of crystal concentration (left) and total crystal size (right) for different number of discretization points.

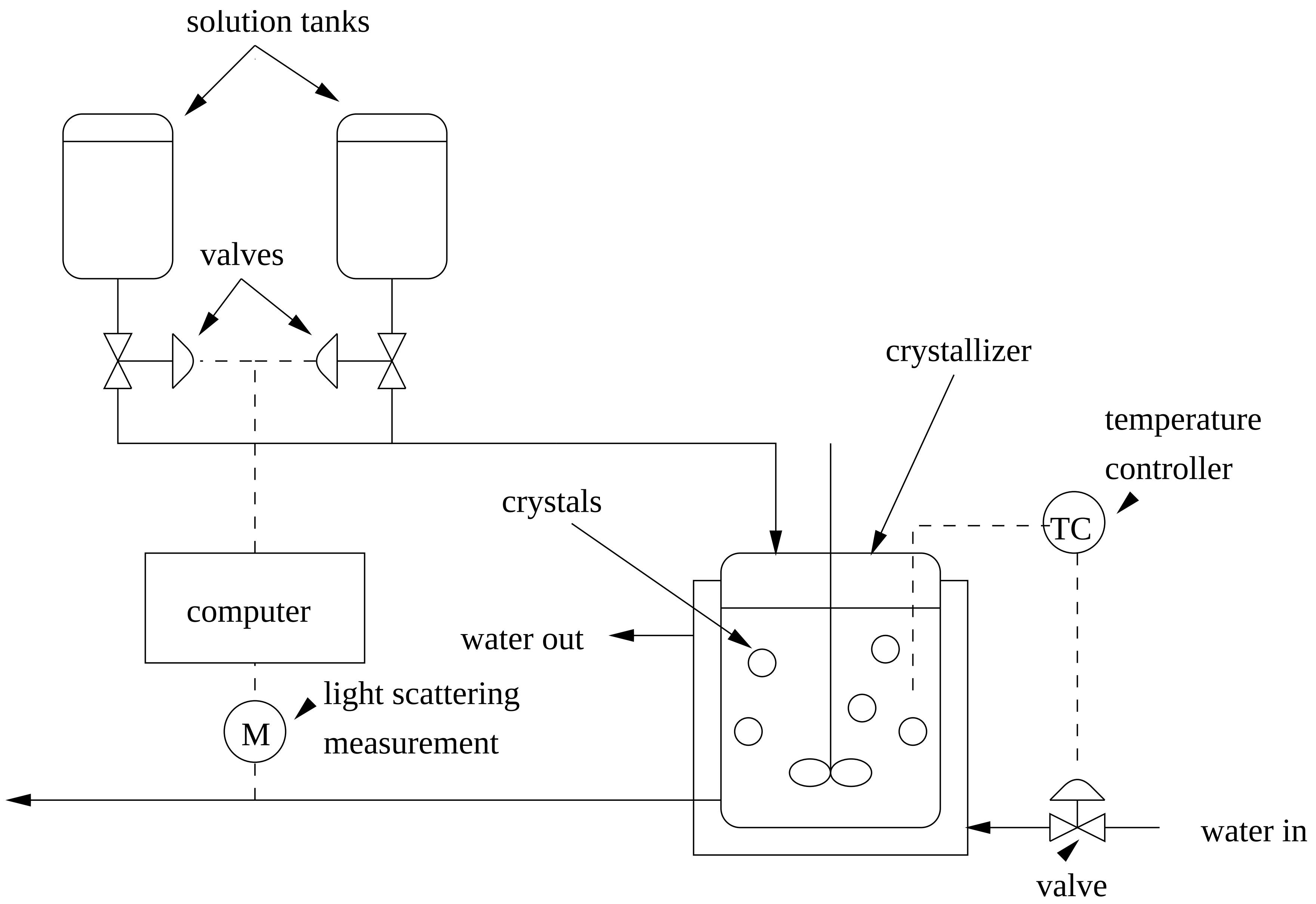




- Feedback control is needed to achieve stabilization.

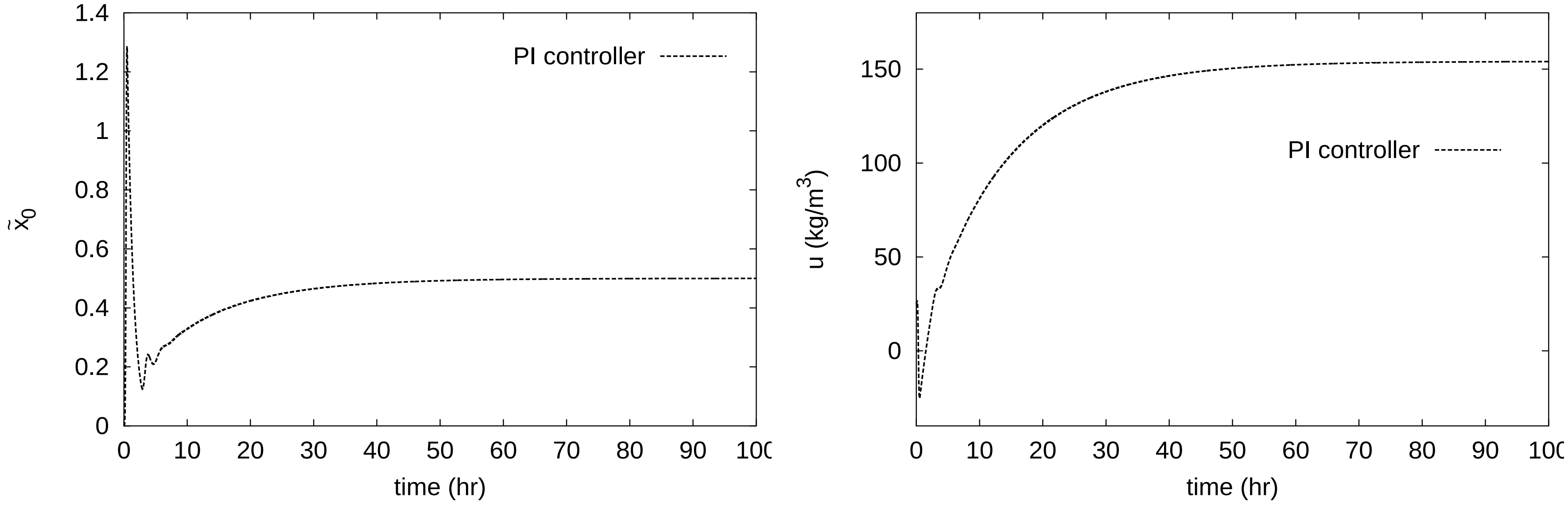
FEEDBACK CONTROL SYSTEM

- Schematic diagram for the continuous crystallizer



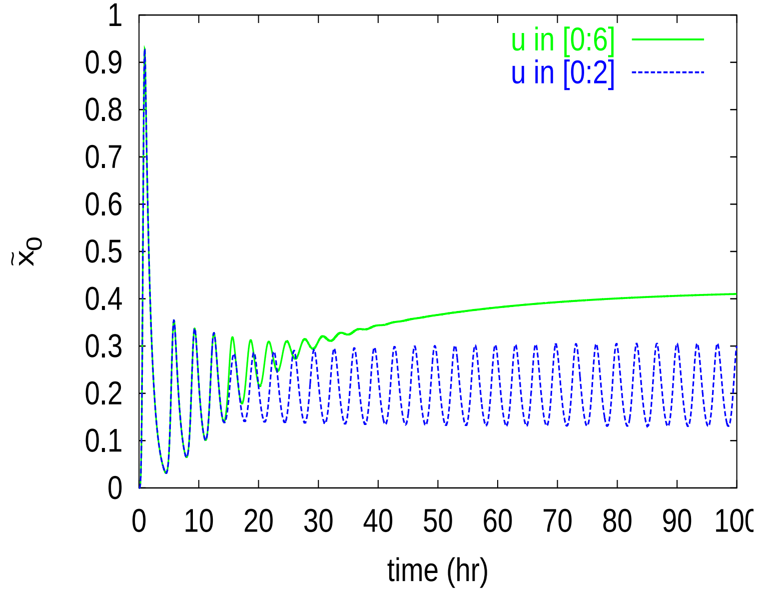
STABILIZATION USING PI CONTROL

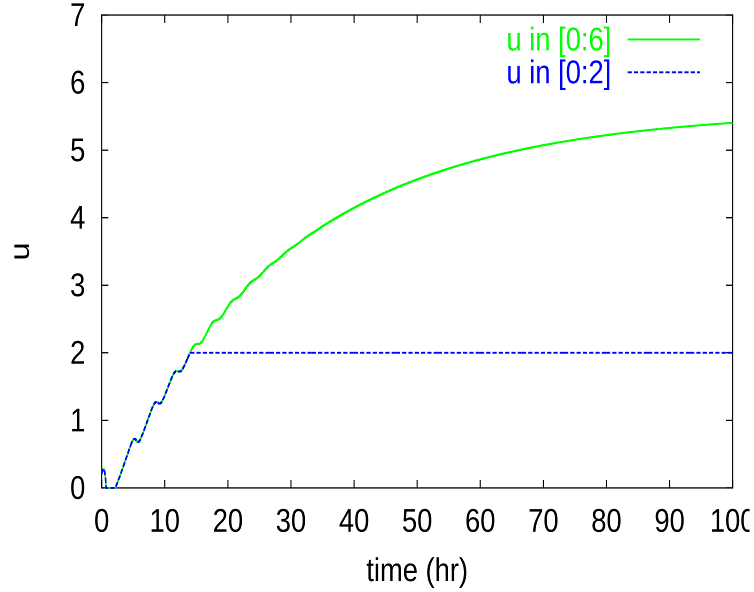
- Closed-loop output (crystal concentration, left figure) and manipulated input (solute concentration, right figure) profiles under PI control, for a 0.5 increase in the set-point ($\tilde{x}_0$ is the controlled output).



STABILIZATION USING CONSTRAINED PI CONTROL

- Closed-loop output (crystal concentration-left) and manipulated input (solute concentration-right) profiles





- Closed-loop instability owing to input constraints.

PARTICULATE PROCESS MODEL

- **Spatially homogeneous process:**
  - ◇ Population balance that describes particle size distribution:

$$\boxed{\frac{\partial \eta}{\partial t} \quad = \quad -\frac{\partial (G(x,r)\eta)}{\partial r} + w(\eta,x,r), \quad \eta(0,t) = b(x(t))}$$

  - ◇ Material and energy balances:

$$\boxed{\dot{x} \quad = \quad f(x) + g(x)u(t) + A\int_0^{r_{max}} a(\eta,r,x)dr}$$

  - ◇ Controlled output:

$$\boxed{y_i(t) \quad = \quad \int_0^{r_{max}} c_i(r)h(\eta(r,t),x)dr}$$

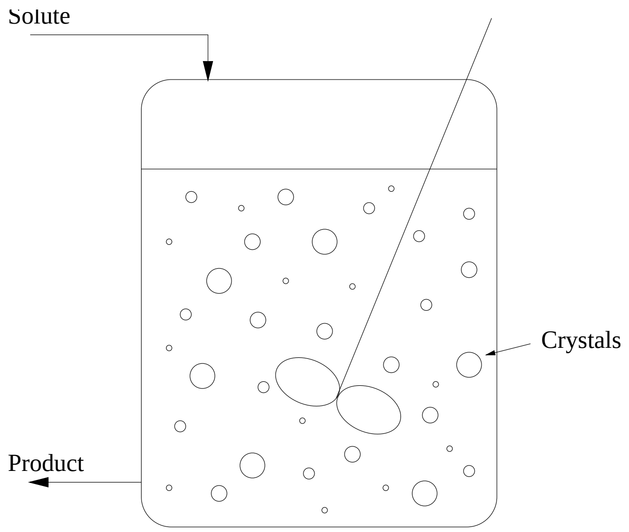
$t \in \mathbb{R}$: time, r : particle size, $\eta \in \mathbb{R}$: particle size distribution.

PARTICULATE PROCESS MODEL

- **Notation:**
  - ◇ $x \in \mathbb{R}^n$: vector of continuous-phase variables.
  - ◇ $u \in \mathbb{R}^m$: manipulated input vector
  - ◇ $y_i \in \mathbb{R}$: controlled output.
  - ◇ $f(x), g(x), b(x(t)), G(x,r), w(\eta, x, r)$: nonlinear functions.
  - ◇ $b(x(t))$: nucleation rate
  - ◇ $G(x,r)$: growth rate.
  - ◇ $w(\eta, x, r)$: breakage/agglomeration processes; product removal.
  - ◇ $A \int_0^{r_{max}} a(\eta, r, x) dr$: Mass transfer rate to all particles in the population - Heat of nucleation/growth.

ISSUES IN PARTICULATE PROCESS CONTROL

- Population balance is a nonlinear distributed parameter system.
  - Not directly suited for controller design.
- Nonlinear behavior:
  - Arrhenius dependence of reaction rates on temperature.
  - Complex reaction mechanisms.
- Model uncertainties:
  - Unknown process parameters.
  - Exogenous disturbances.



Continuous crystallizer

- Input and state constraints:
  - Limited capacity of control actuators.
  - Operating ranges for process variables (environmental, safety, quality constraints).
- Limited process state information
  - Inaccessible states for on-line measurements.

MODEL REDUCTION OF PBMs

- **Population balance model:**

$$\boxed{\begin{aligned}\frac{\partial \eta}{\partial t} &= -\frac{\partial (G(x,r)\eta)}{\partial r} + w(\eta, x, r), \quad \eta(0,t) = b(x(t)) \\ \dot{x} &= f(x) + g(x)u(t) + A\int_0^{r_{max}} a(\eta, r, x)dr\end{aligned}}$$

- **Method of weighted residuals and approximate inertial manifold.**

◇ Step 1: Expansion of $\eta(r,t)$ in an infinite sum

$$\boxed{\eta(r,t) = \sum_{k=1}^{\infty} a_k(t)\phi_k(r)}$$

$a_k(t)$: time-varying coefficients,

$\phi_k(r)$: global basis functions defined on $r \in [0, r_{max}]$.

◇ Step 2: Substituting in the PBM

◇ Step 3: Inner product in $L_2[0, r_{max}]$ with weighting functions $\psi_m(r)$; infinite set of ODEs in time:

MODEL REDUCTION OF PBMs

$$\int_0^{r_{max}} \psi_m(r) \sum_{k=1}^{\infty} \phi_k(r) \frac{\partial a_k(t)}{\partial t} dr = -\sum_{k=1}^{\infty} a_k(t) \int_0^{r_{max}} \psi_m(r) \frac{\partial (G(x,r)\phi_k(r))}{\partial r} dr$$

$$+ \int_0^{r_{max}} \psi_m(r) w(\sum_{k=1}^{\infty} a_k(t)\phi_k(r), x, r) dr, \quad \eta(0,t) = b(x(t))$$

$$m = 0, 1, \ldots, \infty$$

$$\dot{x} = f(x) + g(x)u(t) + A \int_0^{r_{max}} a(\sum_{k=1}^{\infty} a_k(t)\phi_k(r), r, x) dr$$

◇ Step 4: Truncation of the infinite set of ODEs to derive a finite $(n+N)$ set of ODEs:

$$\begin{aligned} \dot{\bar{a}}_k &= \bar{f}(\bar{a}_k, \bar{x}) \\ \dot{\bar{x}} &= f(\bar{x}) + g(\bar{x})u(t) + A \int_0^{r_{max}} a(\sum_{k=1}^{N} \bar{a}_k \phi_k(r), r, \bar{x}) dr \end{aligned}$$

MODEL REDUCTION OF PBMs

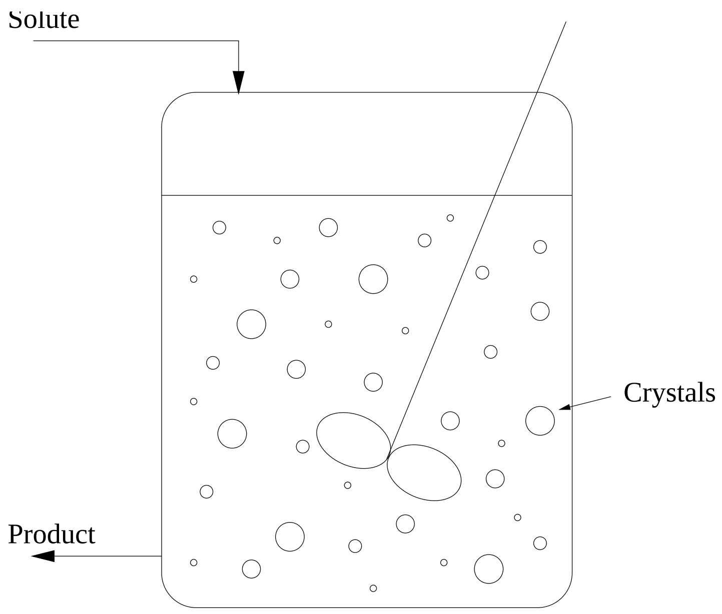
- When $\eta, \dfrac{\partial \eta}{\partial r}$ are continuous and $u(t) \equiv 0$, then for all $t \in [0, \infty)$:

$$\boxed{\lim_{N \to \infty} ||\eta(r,t) - \sum_{k=1}^{N} \bar{a}_k(t)\phi_k(r)||_2 = 0}$$

- When $\psi_m = r^m$: MWR reduces to the method of moments.

- Use of approximate inertial manifolds is possible.

APPLICATION TO A CONTINUOUS CRYSTALLIZER



- Mathematical model:

$$\frac{\partial n}{\partial \bar{t}} = -\frac{\partial (k_1(c - c_s)n)}{\partial r} - \frac{n}{\tau} + \delta(r - 0)\epsilon k_2 exp(-\frac{k_3}{\left(\frac{c}{c_s} - 1\right)^2})$$

$$\frac{dc}{d\bar{t}} = \frac{(c_0 - \rho)}{\bar{\epsilon}\tau} + \frac{(\rho - c)}{\tau} + \frac{(\rho - c)}{\bar{\epsilon}}\frac{d\bar{\epsilon}}{d\bar{t}}$$

MODEL REDUCTION OF CONTINUOUS CRYSTALLIZER

- **Method of moments:**

$$\boxed{m_j = \int_0^\infty r^j n(r,t)dr, \quad j = 0, \ldots, \infty}$$

- **Infinite set of ODEs:**

$$\begin{aligned}
\frac{dm_0}{dt} &= -\frac{m_0}{\tau} + \left(1 - \frac{4}{3}\pi m_3\right) k_2 e^{-\frac{k_3}{\left(\frac{c}{c_s} - 1\right)^2}} \\
\frac{dm_j}{dt} &= -\frac{m_j}{\tau} + jk_1(c - c_s)m_{j-1}, \quad j = 1, 2, 3, \ldots, \infty \\
\frac{dc}{dt} &= \frac{c_0 - c - 4\pi\tau(c - c_s)m_2(\rho - c)}{\tau\left(1 - \frac{4}{3}\pi m_3\right)}
\end{aligned}$$

MODEL REDUCTION OF CONTINUOUS CRYSTALLIZER

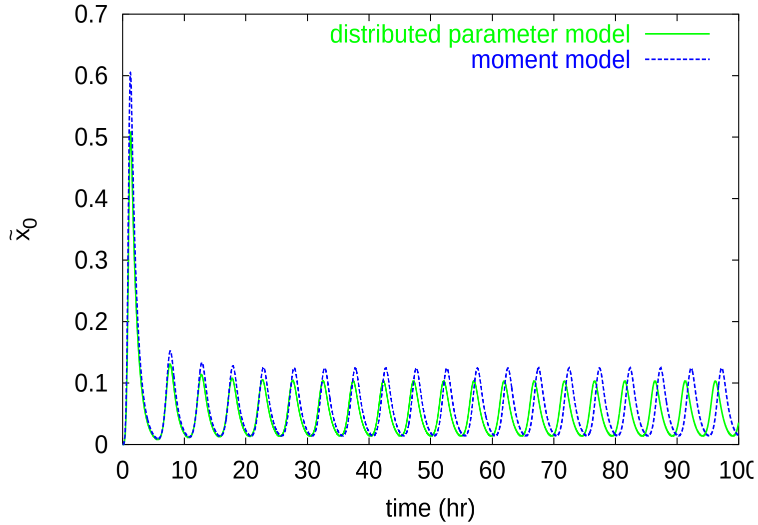
- **Finite set (1+4) of ODEs:**

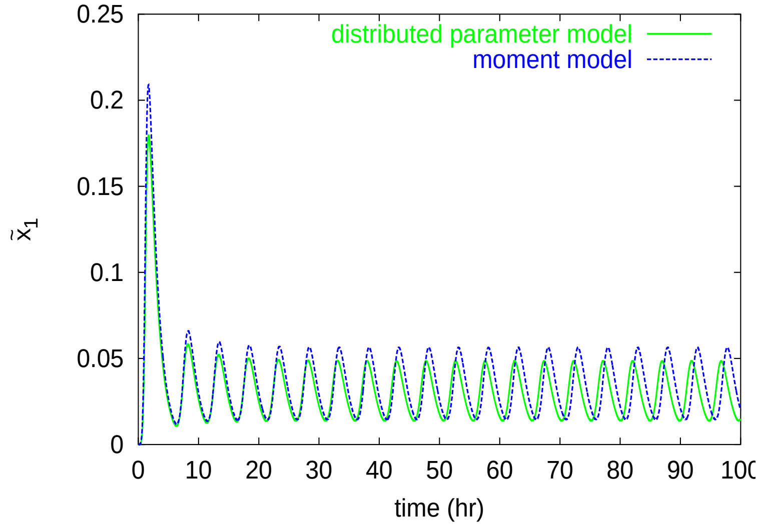
$$\boxed{\begin{aligned}
\frac{dm_0}{dt} &= -\frac{m_0}{\tau} + \left(1 - \frac{4}{3}\pi m_3\right) k_2 e^{-\frac{k_3}{\left(\frac{c}{c_s} - 1\right)^2}} \\
\frac{dm_j}{dt} &= -\frac{m_j}{\tau} + j k_1 (c - c_s) m_{j-1}, \quad j = 1, 2, 3 \\
\frac{dc}{dt} &= \frac{c_0 - c - 4\pi\tau(c - c_s) m_2 (\rho - c)}{\tau\left(1 - \frac{4}{3}\pi m_3\right)}
\end{aligned}}$$

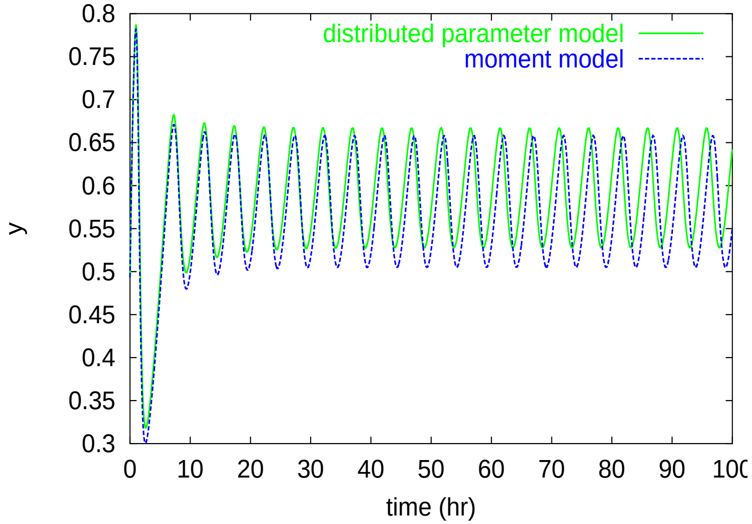
- **Dominant dynamics are low-dimensional.**

OPEN-LOOP BEHAVIOR PREDICTED BY DISTRIBUTED PARAMETER AND MOMENT MODELS

- Open-loop profiles of crystal concentration (left), total crystal size (right), and solute concentration (bottom).

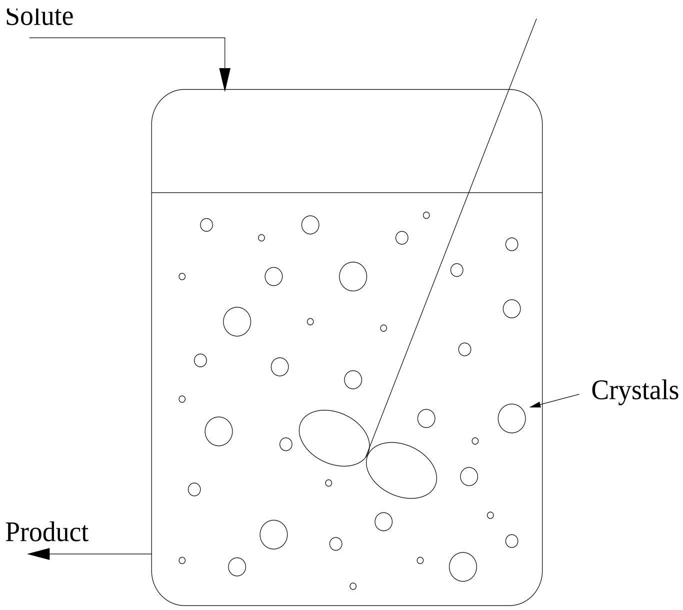






CONTINUOUS CRYSTALLIZATION

Control problem specification



- Mathematical model:

$$\frac{\partial n}{\partial \bar{t}} = -\frac{\partial(k_1(c-c_s)n)}{\partial r} - \frac{n}{\tau} + \delta(r-0)\epsilon k_2 exp(-\frac{k_3}{\left(\frac{c}{c_s}-1\right)^2})$$

$$\frac{dc}{d\bar{t}} = \frac{(c_0-\rho)}{\bar{\epsilon}\tau} + \frac{(\rho-c)}{\tau} + \frac{(\rho-c)}{\bar{\epsilon}}\frac{d\bar{\epsilon}}{d\bar{t}}$$

- Control problem: $u(t) = c_0 - c_{0s}$, $y(t) = \int_0^\infty n(r,t)dt.$

GEOMETRIC NONLINEAR CONTROL

$$\boxed{\begin{aligned} \frac{dx}{dt} &= f(x) + g(x)u \\ y &= h(x) \end{aligned}}$$

- **Feedback linearization:**
  - ◇ Controller synthesis formula

$$u = \frac{1}{L_g L_f^{r-1} h(x)} \left(v - L_f^r h(x) - \sum_{k=1}^{r} \beta_k L_f^{r-k} h(x) \right)$$

Lie derivative notation: $L_f h(x) = \frac{\partial h}{\partial x} f(x)$.

  - ◇ Input/Output Dynamics

$$\frac{d^r y}{dt} + \beta_1 \frac{d^{r-1} y}{dt} + \cdots + \beta_{r-1} \frac{dy}{dt} + \beta_r y = v$$

$\beta_1, \cdots, \beta_r$ are tuning parameters (time constants).

- **Nonlinear state estimator design:**
  - ◇ Nonlinear Luenberger-type state estimator.

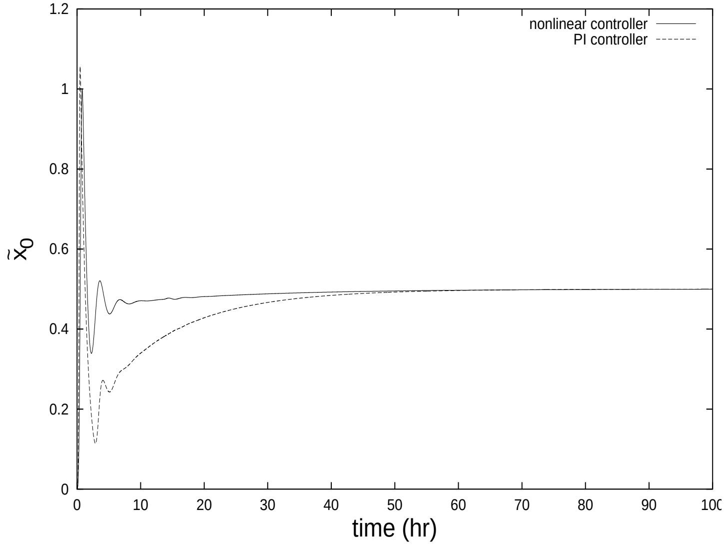
$$\frac{d\eta}{dt} = f(\eta) + g(\eta)u + L(y - h(\eta))$$

  - ◇ L: observer gain.

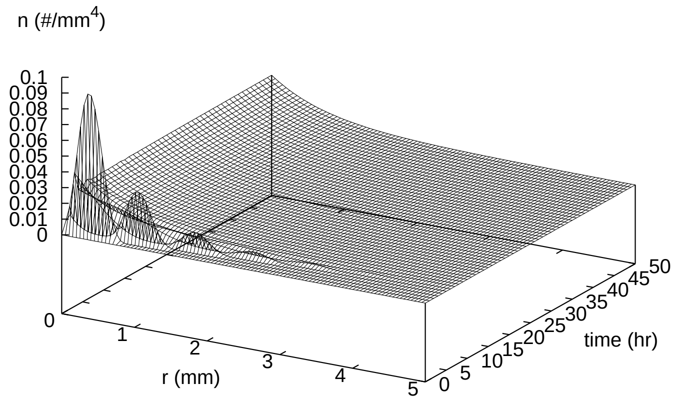
CONTINUOUS CRYSTALLIZATION

Closed-loop simulation results

Closed-loop output profile under nonlinear and PI control.



Closed-loop crystal size distribution under nonlinear control.



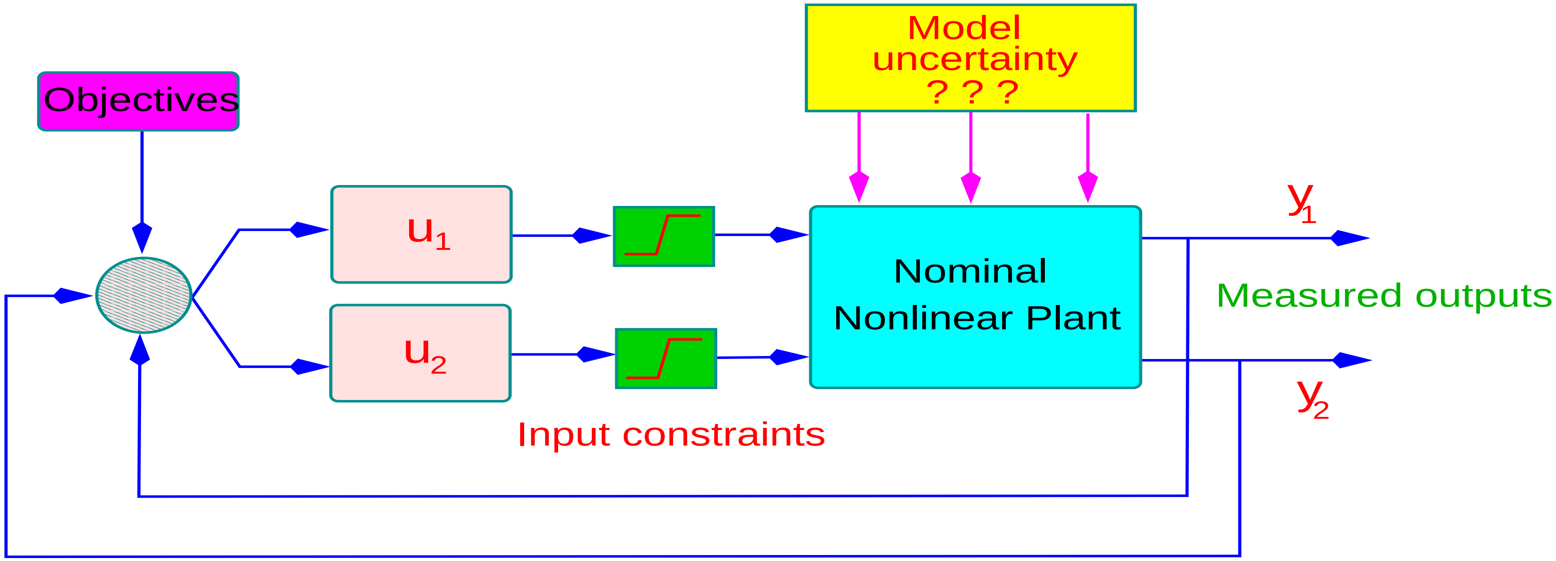
ADVANCED MODEL-BASED NONLINEAR CONTROL

- **State space description:**

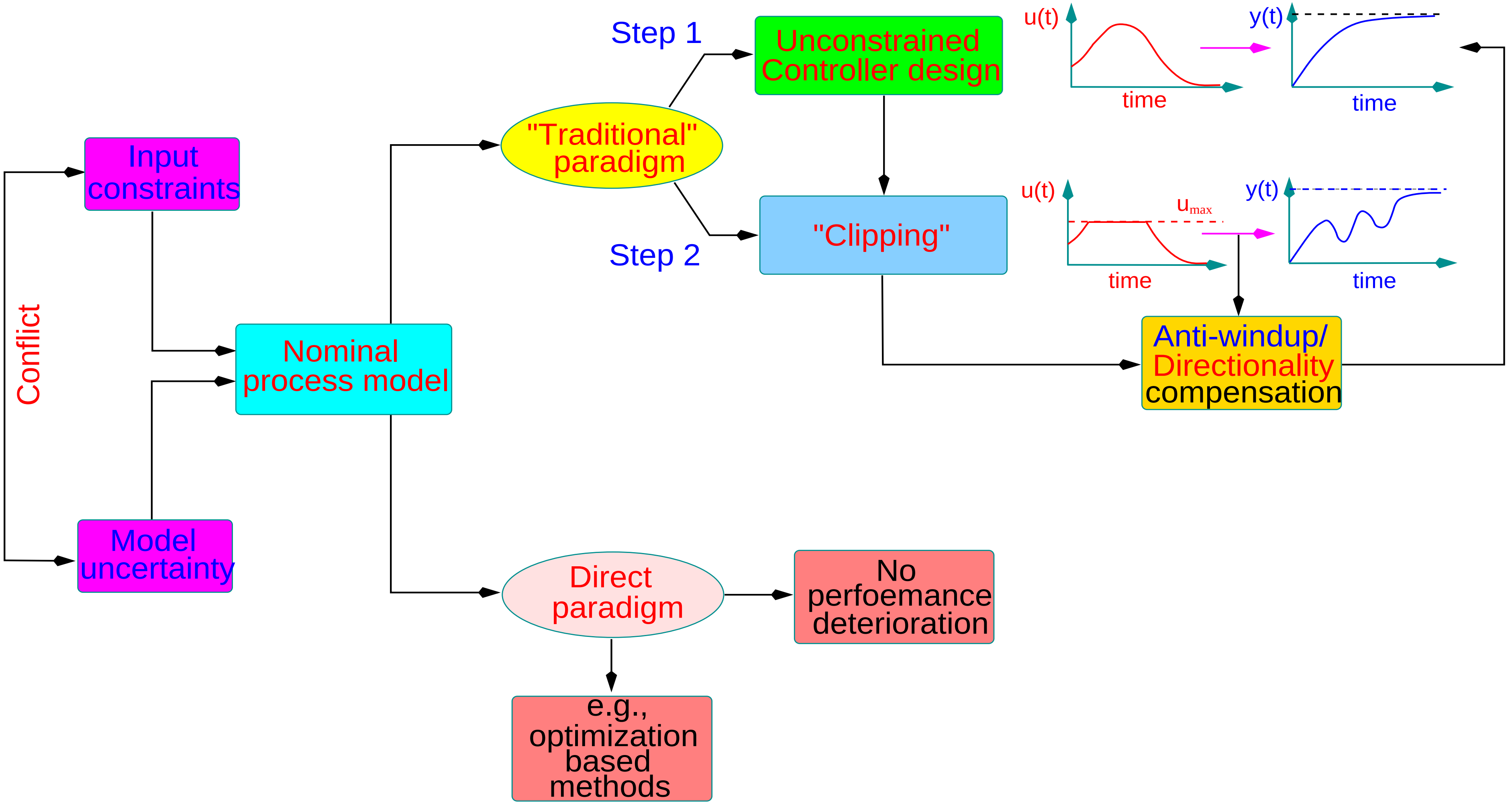
$$\begin{aligned}
\dot{x} &= f(x) + \sum_{i=1}^{m} g_i(x)u_i + \sum_{k=1}^{q} w_k(x)\theta_k(t) \\
y_i &= h_i(x), \quad i = 1, \cdots, m
\end{aligned}$$

$$u_{i_{min}} \leq u_i \leq u_{i_{max}}$$

- ◇ $x \in \mathbb{R}^n$: process states
- ◇ $u_i \in \mathcal{U} \subset \mathbb{R}$: manipulated inputs
- ◇ $y_i \in \mathbb{R}$: controlled outputs
- ◇ $\theta_k \in \mathcal{W} \subset \mathbb{R}$: uncertain variables



CONTROL PARADIGMS FOR CONSTRAINED UNCERTAIN NONLINEAR SYSTEMS



- **Issues of practical implementation:**
  - ◇ Computational complexity
  - ◇ Characterizing closed-loop stability properties
  - ◇ Robustness to constant and time-varying uncertainty

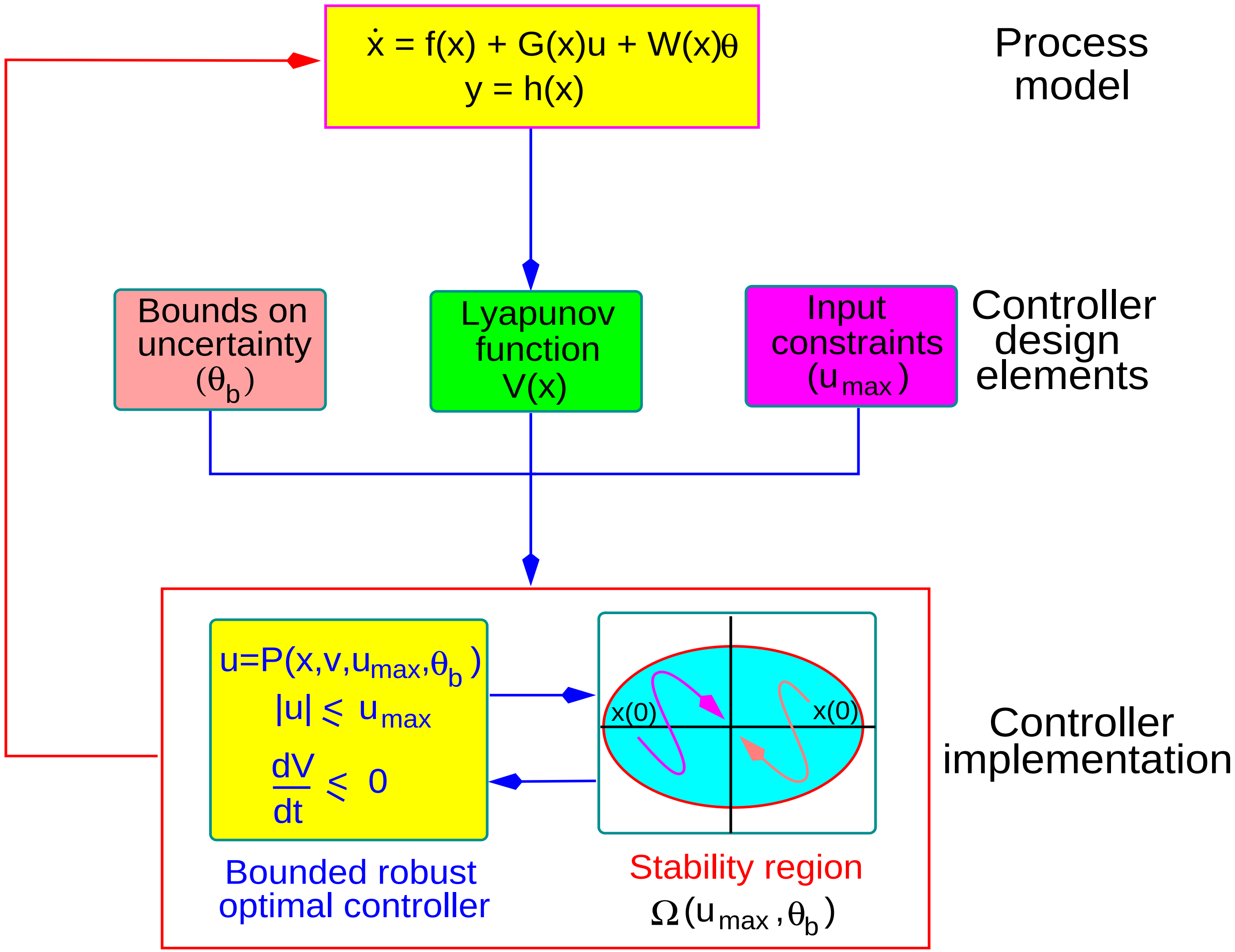
BOUNDED ROBUST OPTIMAL CONTROL

(El-Farra and Christofides, Chem. Eng. Sci., 2001; 2003)

- **Basic conceptual tools:**
  - ◇ Lyapunov theory
  - ◇ Bounded control
  - ◇ Inverse optimal control theory
- **Integrated framework for nonlinear control:**
  - ◇ Robust stability
    - ⋆ Arbitrary degree of attenuation of plant-model mismatch
  - ◇ Optimality
    - ⋆ Avoids wasteful cancellation of process nonlinearities
  - ◇ Explicit constraint-handling
    - ⋆ Avoids performance deterioration
  - ◇ Explicit characterization of stability region
    - ⋆ A priori knowledge of feasible initial conditions

BOUNDED ROBUST OPTIMAL CONTROL

(El-Farra and Christofides, Chem. Eng. Sci., 2001; 2003)



⋆ **Multivariable interactions**

⋆ **Accessibility of process states for measurement**

NONLINEAR CONTROLLER SYNTHESIS

- Constrained low-order ODE system:

$$\boxed{\begin{aligned} \dot{\bar{a}}_k &= \bar{f}(\bar{a}_k, \bar{x}), \ u \in [u_{min}, u_{max}] \\ \dot{\bar{x}} &= f(\bar{x}) + g(\bar{x})u(t) + A\int_0^{r_{max}} a(\sum_{k=1}^{N} \bar{a}_k \phi_k(r), r, \bar{x})dr \end{aligned}}$$

- State feedback controller synthesis:
  - ◇ Bounded Lyapunov-based control law

$$\boxed{u \quad = \quad -\frac{1}{2}R^{-1}(\tilde{x})L_{\bar{g}}V}$$

  - ◇ Closed-loop properties under active input constraints
    - ▷ Exponential stability / Asymptotic set-point tracking
    - ▷ Optimality
  - ◇ Explicit characterization of the region of closed-loop stability.

$$\boxed{L_{\bar{f}}V \quad \leq \quad u_{max}|L_{\bar{g}}V|}$$

OUTPUT FEEDBACK IMPLEMENTATION

- Combination of state feedback with state observer:
  - ◇ State observer: nonlinear Luenberger-type observer.
  - ◇ Nonlinear output feedback controller.

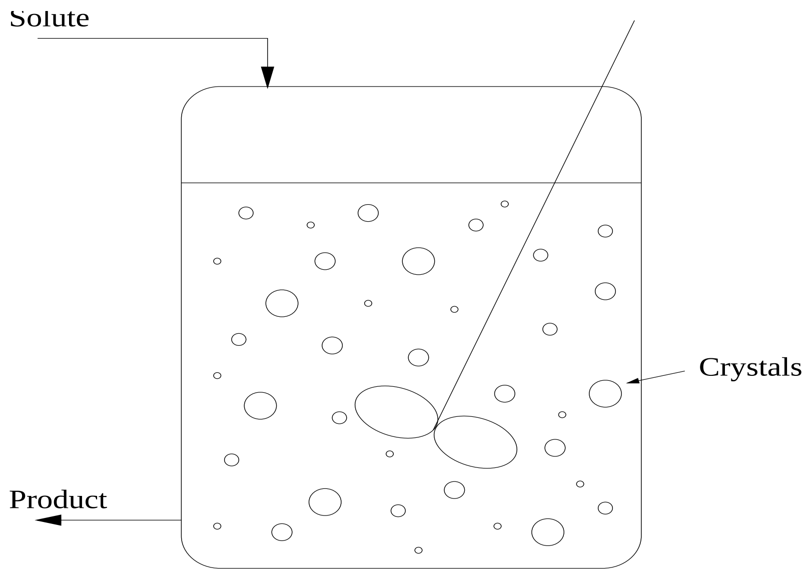
$$\boxed{\begin{array}{rcl} \dot{w} & = & \tilde{f}(\omega) + \tilde{g}(\omega)u + L(y - \tilde{h}(\omega)) \\ u & = & -\dfrac{1}{2}R^{-1}(\omega)L_{\bar{g}}V \end{array}}$$

where ω is the estimate of $\tilde{x}$.

- Closed-loop stability region practically preserved for large observer gain.

- Exponential stability of constrained closed-loop ODE system implies exponential stability of constrained closed-loop DPS.

APPLICATION TO A CONTINUOUS CRYSTALLIZER



- **Process model:**

$$
\boxed{
\begin{aligned}
\frac{\partial n}{\partial t} &= -k_1(c-c_s)\frac{\partial n}{\partial r} - \frac{n}{\tau} + \delta(r-0)\epsilon k_2 e^{-\frac{k_3}{\left(\frac{c}{c_s}-1\right)^2}} \\
\frac{dc}{dt} &= \frac{(c_0-\rho)}{\epsilon\tau} + \frac{(\rho-c)}{\tau} + \frac{(\rho-c)}{\epsilon}\frac{d\epsilon}{dt}
\end{aligned}
}
$$

- **Control problem:**

$$
\boxed{u(t) = c_0, \quad y(t) = \int_0^\infty \eta(r,t)dr}
$$

COMPUTATION OF ADMISSIBLE SET-POINTS

- Small set of algebraic equations:

$$\boxed{\begin{aligned} 0 &= \bar{f}(\bar{a}_k, \bar{x}) \\ 0 &= f(\bar{x}) + g(\bar{x})u(t) + A\int_0^{r_{max}} a(\sum_{k=1}^{N} \bar{a}_k \phi_k(r), r, \bar{x})dr, \\ & u \in U = [u_{min}, u_{max}] \end{aligned}}$$

- Computation of all equilibrium points for $u \in U$ using approximate model.

$$\boxed{D = \{(\bar{a}_{ks}, \bar{x}_s), \ \forall \ u^0 \in U\}}$$

- Computation of admissible set-points.

$$\boxed{v_i = \int_0^{r_{max}} c_i(r)h(\sum_{k=1}^{N} \bar{a}_{ks}\phi_k(r), \bar{x}_s)dr}$$

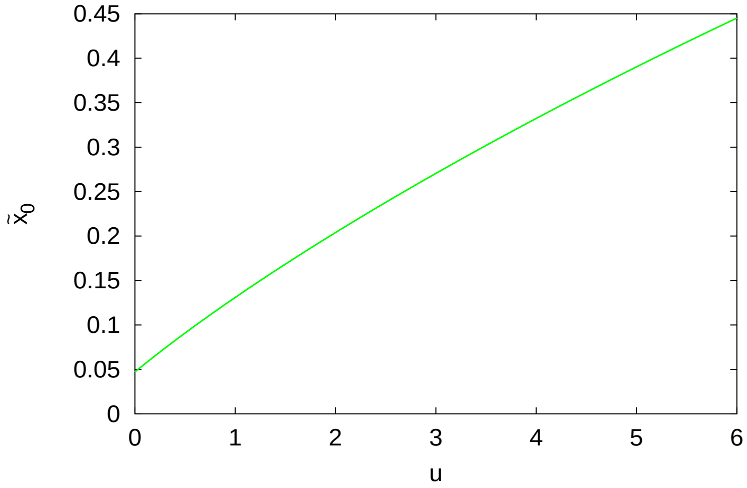
- Straightforward computation; approximate set-points for the population balance model.

COMPUTATION OF ADMISSIBLE SET-POINTS

- Steady-state moment model in dimensionless form:

$$\boxed{\begin{aligned}
0 &= -\tilde{x}_{0_s} + (1-\tilde{x}_{3_s})Dae^{\frac{-F}{\tilde{y}_s^2}} \\
0 &= -\tilde{x}_{1_s} + \tilde{y}_s\tilde{x}_{0_s} \\
0 &= -\tilde{x}_{2_s} + \tilde{y}_s\tilde{x}_{1_s} \\
0 &= -\tilde{x}_{3_s} + \tilde{y}_s\tilde{x}_{2_s} \\
0 &= \frac{1-\tilde{y}_s-(\alpha-\tilde{y}_s)\tilde{y}_s\tilde{x}_{2_s}}{1-\tilde{x}_{3_s}} + \frac{u}{1-\tilde{x}_{3_s}}
\end{aligned}}$$

- Set of admissible set-points for $u \in [0, 6]$



NONLINEAR CONTROLLER DESIGN

- Model reduction via method of moments:

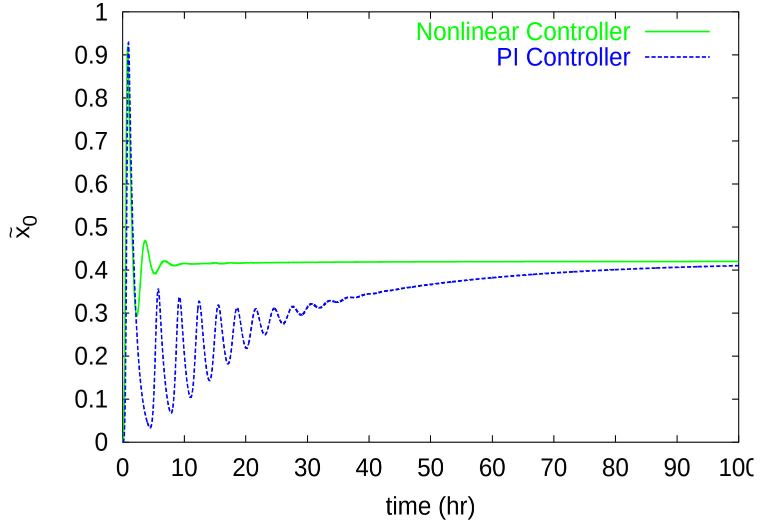
$$\boxed{m_j \quad = \quad \int_0^\infty r^j n(r,t)dr, \;\; j = 0, \ldots, \infty}$$

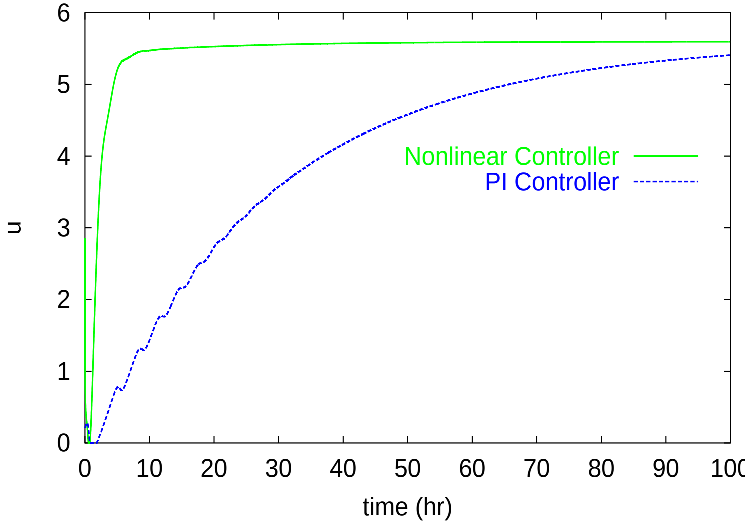
- Finite set (1+4) of ODEs.
- Nonlinear output feedback controller:

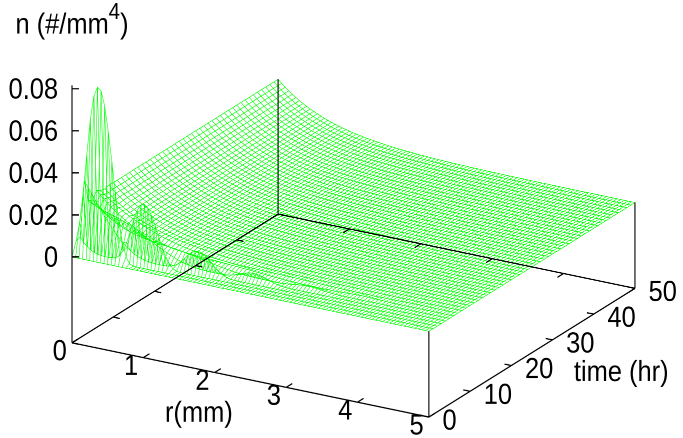
$$\boxed{\begin{aligned}
\frac{d\omega_0}{dt} &= -\omega_0 + (1-\omega_3)Dae^{\frac{-F}{\omega_4^2}} + L_1(x_0 - \omega_0) \\
\frac{d\omega_j}{dt} &= -\omega_j + \omega_4\omega_{j-1}, \;\; j = 1,2,3 \\
\frac{d\omega_4}{dt} &= \frac{1-\omega_4-(\alpha-\omega_4)\omega_4\omega_2}{1-\omega_3} + L_5(x_0-\omega_0) + \\
&\quad + \frac{u(t)}{1-\omega_3} \\
u(t) &= -\frac{1}{2}R^{-1}(\omega)L_{\bar{g}}V
\end{aligned}}$$

CLOSED-LOOP SIMULATION RESULTS

- Controlled output (left), manipulated input (right) and crystal size distribution (bottom) profiles.



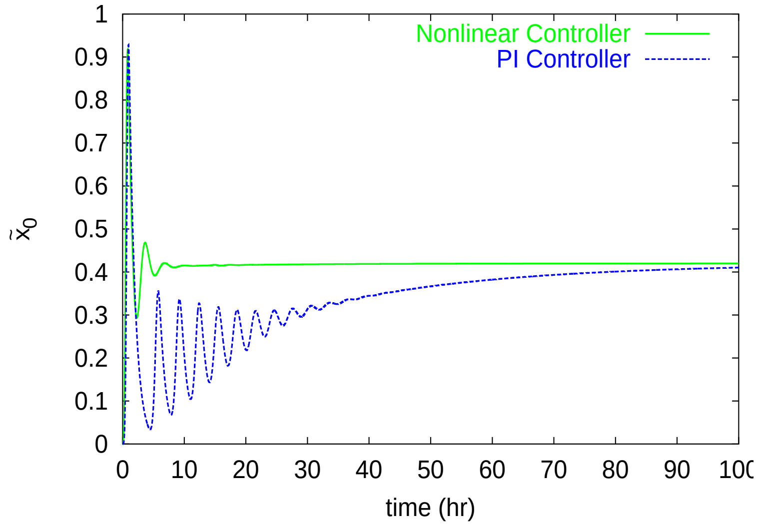


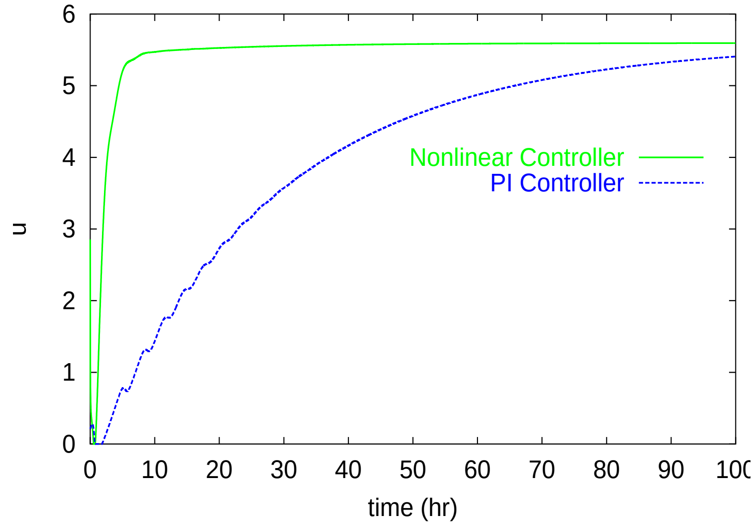


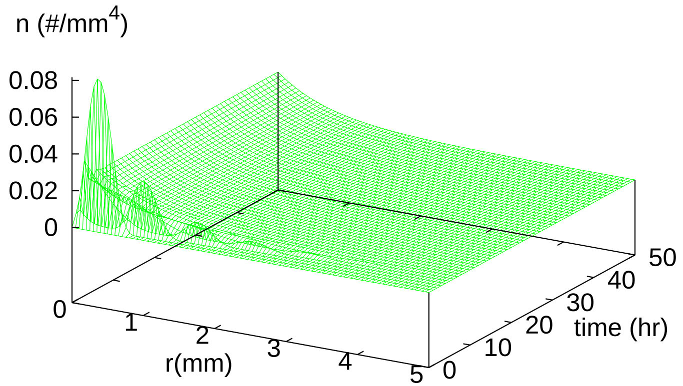
CLOSED-LOOP SIMULATION RESULTS

Parametric uncertainty

- Controlled output (left), manipulated input (right) and crystal size distribution (bottom) profiles.



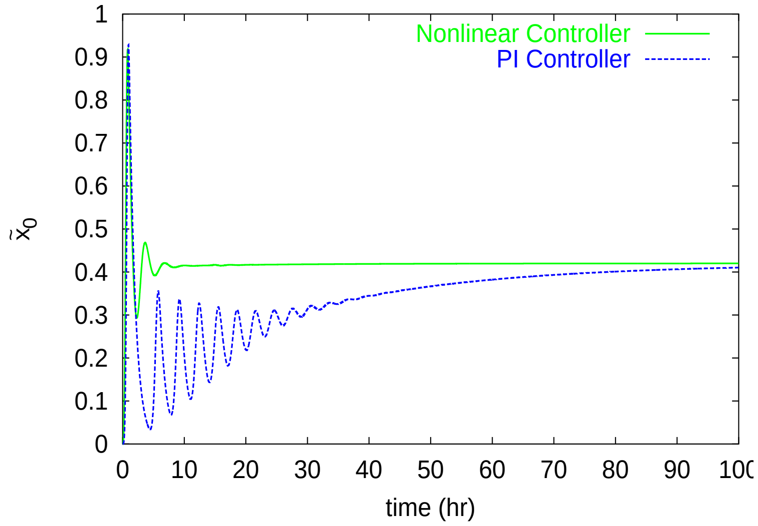


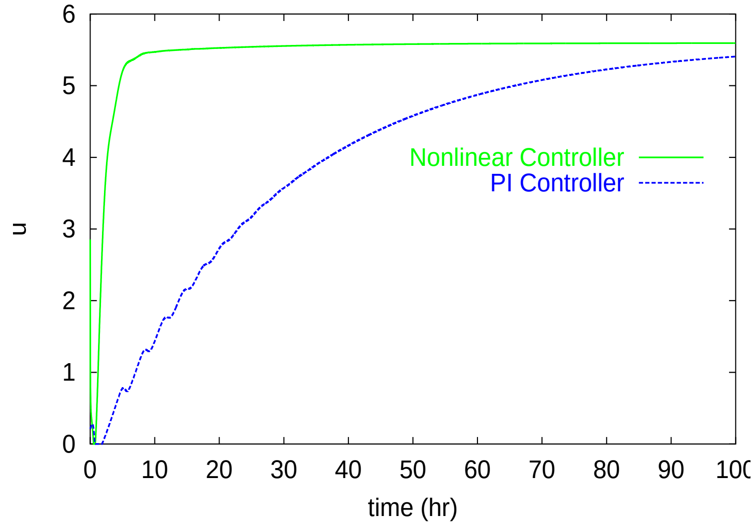


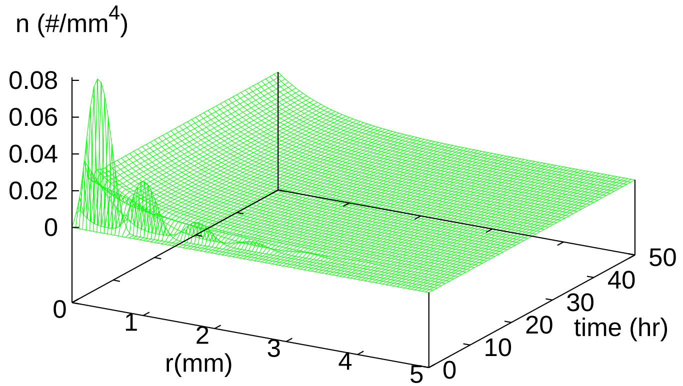
CLOSED-LOOP SIMULATION RESULTS

Unmodeled actuator/sensor dynamics

- Controlled output (left), manipulated input (right) and crystal size distribution (bottom) profiles.







NONLINEAR CONTROL THEORY VS. PROCESS CONTROL PRACTICE

- Nonlinear control theory and tools:
  - ◇ Require thorough understanding of the process ('sufficiently' accurate process models).
  - ◇ Geometric control, Lyapunov-based control, feedback linearization, etc.
  - ◇ Allow rigorous analysis of closed–loop stability and performance properties.
- Process control practice:
  - ◇ Proportional Integral Derivative (PID) controllers, Linear Model Predictive Control (MPC).
  - ◇ Do not account for the complex dynamics of the process.
- Nonlinear control implementation requires **redesign** of control hardware:

$$\boxed{\text{Use nonlinear control theory to aid process control practice}}$$

NONLINEAR SYSTEMS WITH INPUT CONSTRAINTS

- **State–space description:**

$$\boxed{\begin{aligned} \dot{x}(t) &= f(x(t)) + g(x)u(t) \\ u(t) &\in \mathcal{U} \end{aligned}}$$

◇ $x(t) \in \mathbb{R}^n$: state vector

◇ $u(t) \in \mathcal{U} \subset \mathbb{R}^m$: control input

◇ $\mathcal{U} \subset \mathbb{R}^m$: compact & convex

◇ $u = 0 \in$ interior of $\mathcal{U}$

◇ $(0,\ 0)$ an equilibrium point

- **Stabilization of origin under constraints**

MODEL PREDICTIVE CONTROL

- **Control problem formulation**

  ◇ Finite-horizon optimal control:

$$P(x,t) \quad : \quad \min\{J(x,t,u(\cdot)) \mid u(\cdot) \in U_\Delta\}$$

  ◇ Performance index:

$$J(x,t,u(\cdot)) \quad = \quad F(x(t+T)) + \int_t^{t+T} \left[\|x^u(s;x,t)\|_Q^2 + \|u(s)\|_R^2 \right] ds$$

▷ $\|\cdot\|_Q$: weighted norm

▷ T : horizon length

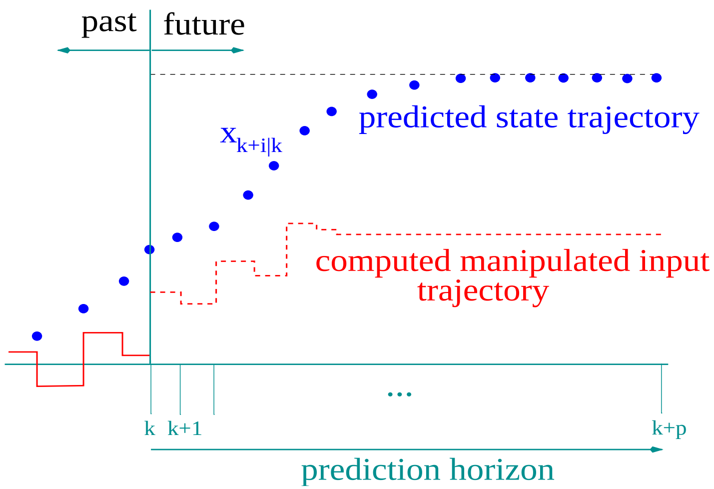
▷ $Q,\ R > 0$: penalty weights

▷ $F(\cdot)$: terminal penalty

  ◇ Implicit feedback law

$$M(x) \quad = \quad u^0(t;x,t)$$

"repeated on-line optimization"



MODEL PREDICTIVE CONTROL

- **Formulations for closed-loop stability:**

  (Mayne et al, Automatica, 2000)

  - ◇ Adjusting horizon length, terminal penalty, weights, etc.
  - ◇ Imposing stability constraints on optimization:
    - ▷ Terminal equality constraints: $\boxed{x(t+T) \;=\; 0}$

- **Issues of practical implementation:**

  - ◇ Optimization problem non-convex
    - ▷ Possibility of multiple, local optima
    - ▷ Optimization problem hard to solve (e.g., algorithm failure)
    - ▷ Difficult to obtain solution within “reasonable” time
  - ◇ Lack of explicit characterization of stability region
    - ▷ Extensive closed-loop simulations
    - ▷ Restrict implementation to small neighborhoods

LYAPUNOV-BASED CONTROL

- **Explicit nonlinear control law:**

$$\boxed{u_\sigma \quad = \quad -k(x, u_{max})(L_{g_\sigma} V)^T}$$

  ◇ Example: bounded controller (Lin & Sontag, 1991)

  ▷ Controller design accounts for constraints.

- **Explicit characterization of stability region:**

$$\boxed{\Omega_\sigma(u_{max}) \quad = \quad \{x \in \mathbb{R}^n : V_\sigma(x) \leq c_\sigma^{max} \ \& \ \dot{V}_\sigma(x) < 0\}}$$

  ◇ Larger estimates using a combination of several Lyapunov functions

UNITING BOUNDED CONTROL AND MPC

(El-Farra, Mhaskar & Christofides, Automatica, 2004; IJRNC, 2004)

- **Objectives:**
  - ◇ Development of a framework for merging the two approaches:
    - ▷ Reconcile tradeoffs in stability and optimality properties
    - ▷ Explicit characterization of constrained stability region
    - ▷ Possibility of improved performance
    - ▷ Implement computationally inexpensive MPC formulations

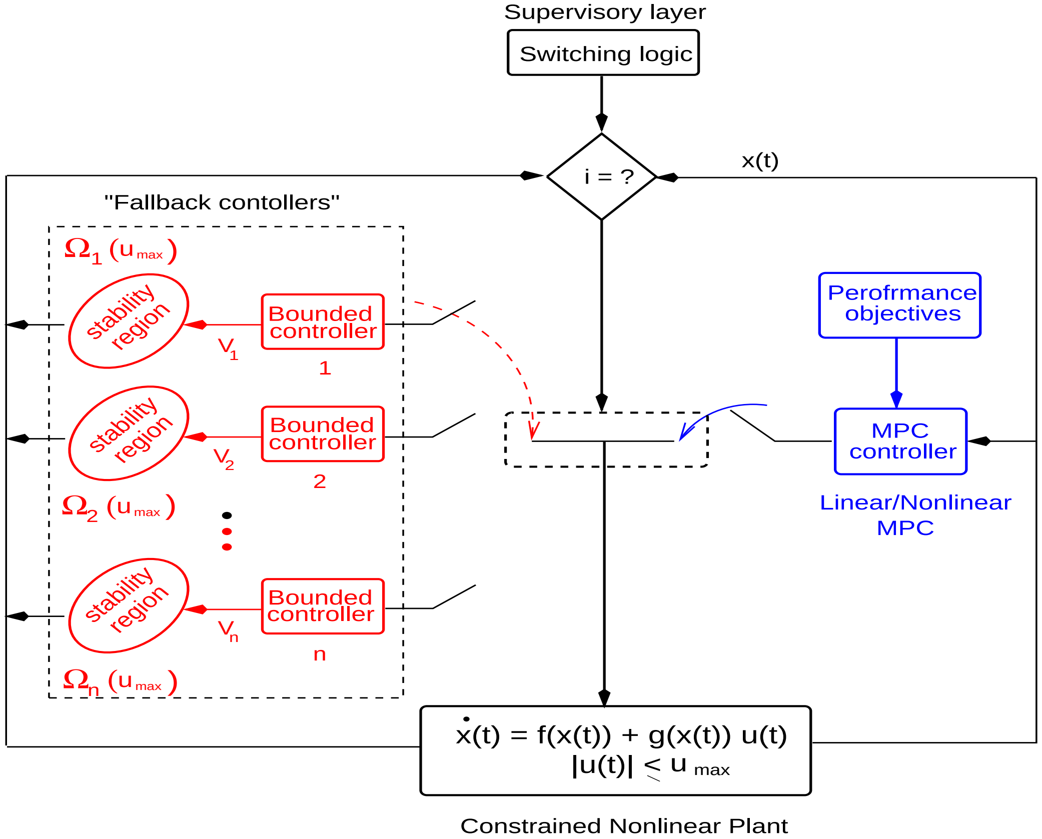
- **Central idea:**

  Decoupling "optimality" & "constrained stabilizability"

  - ◇ Stability region provided by bounded controller
  - ◇ Optimal performance supplied by MPC controller

- **Approach:**
  - ◇ Switching between MPC & a family of bounded controllers

OVERVIEW OF HYBRID CONTROL STRATEGY



- **Hierarchical control structure**
  - ◇ Plant level ◇ Control level ◇ Supervisory level
- Overall structure **independent** of specific MPC algorithm used
  - ◇ Could use linear/nonlinear MPC with or without stability constraints

STABILITY-BASED CONTROLLER SWITCHING

- **Switching logic:**

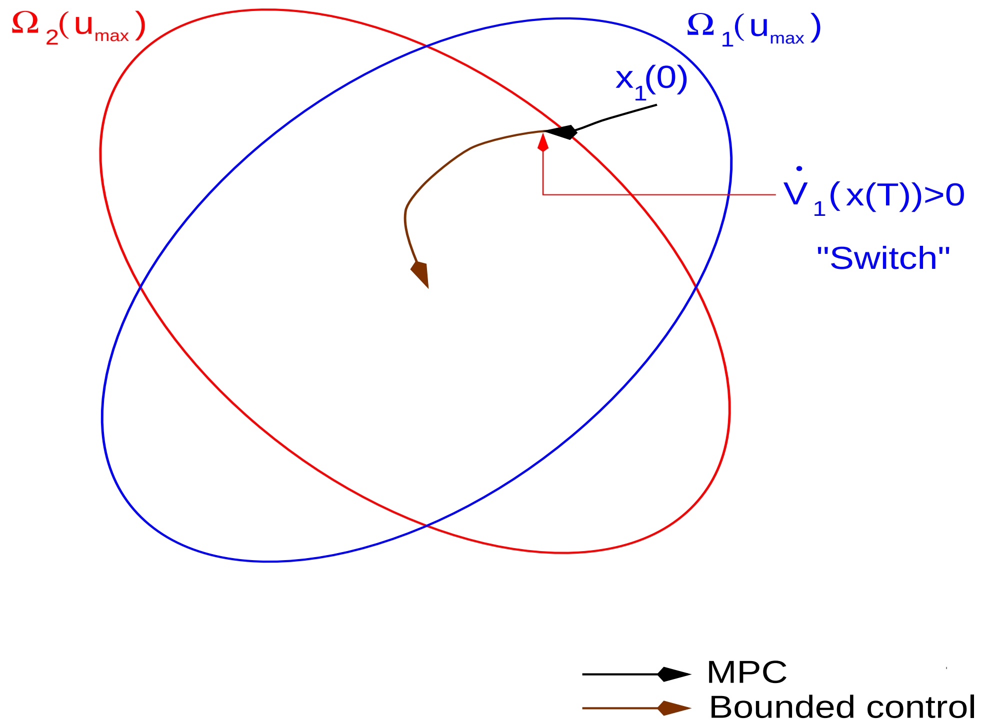
$$u_\sigma(x(t)) \quad = \quad \left\{ \begin{array}{ll} M(x(t)), & 0 \leq t < T^* \\ b(x(t)), & t \geq T^* \end{array} \right\}$$

$$L_f V_k(x) + L_g V_k(x) M(x(T^*)) \geq 0$$

◇ Initially implement MPC, $x(0) \in \Omega_k(u_{max})$

◇ Monitor temporal evolution of $V_k(x^M(t))$

◇ Switch to bounded controller only if $V_k(x^M(t))$ starts to increase



IMPLICATIONS OF SWITCHING SCHEME

- Switched closed-loop inherits bounded controller's stability region
  - ◇ A priori guarantees for all $x(0) \in \Omega(u_{max})$
- Lyapunov stability condition checked & enforced by "supervisor"
  - ◇ Reduce computational complexity of optimization
  - ◇ Scheme does not require stability of MPC within $\Omega(u_{max})$
  - ◇ Provides a safety net for implementing MPC
  - ◇ Stability independent of horizon length
- Conceptual differences from other schemes:
  - ◇ Switching does not occur locally
  - ◇ Provides stability region explicitly
  - ◇ No switching occurs if $V(x^M(t))$ decays continuously
    - ▷ Only MPC is implemented $\Longrightarrow$ optimal performance recovered

PREDICTIVE CONTROL IN INDUSTRIAL PRACTICE

- A "typical" predictive control design:
  - ◇ Nonlinear process model:

$$\boxed{\begin{aligned} \dot{x} &= f(x) + g(x)u \\ u_{min}^i \leq u_i &\leq u_{max}^i \end{aligned}}$$

  - ◇ Linear representation:

$$\boxed{\begin{aligned} \dot{x} &= Ax + Bu \\ u_{min}^i \leq u_i &\leq u_{max}^i \end{aligned}}$$

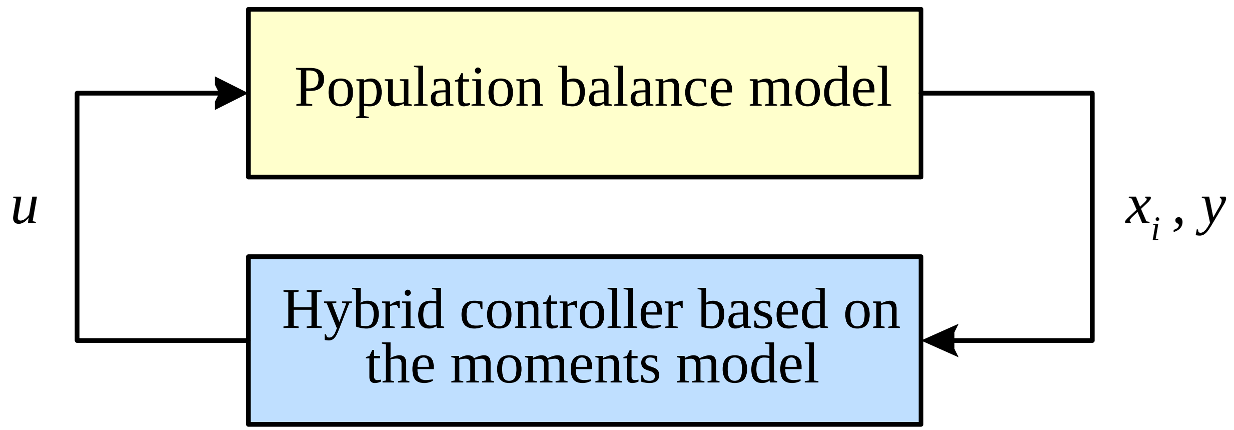
    - ⋆ Linearization (around desired steady-state)
    - ⋆ Model identification (e.g., through step tests)
  - ◇ Use of computationally efficient linear MPC (QP) algorithms
  - ◇ No closed-loop stability guarantees for nonlinear system
- Practical value of the hybrid control structure:
  - ◇ Provides stability guarantees through fall-back controllers
  - ◇ Entails no modifications in existing predictive controller design

APPLICATION TO A CONTINUOUS CRYSTALLIZER

- **Population balance model:**

$$\boxed{\begin{aligned} \frac{\partial n}{\partial t} &= -k_1(c-c_s)\frac{\partial n}{\partial r} - \frac{n}{\tau} + \delta(r-0)\epsilon k_2 e^{-\frac{k_3}{\left(\frac{c}{c_s}-1\right)^2}} \\ \frac{dc}{dt} &= \frac{(c_0-\rho)}{\epsilon\tau} + \frac{(\rho-c)}{\tau} + \frac{(\rho-c)}{\epsilon}\frac{d\epsilon}{dt} \end{aligned}}$$

- **Hybrid control loop structure:**



APPLICATION TO A CONTINUOUS CRYSTALLIZER

- **Crystallizer moments model:**

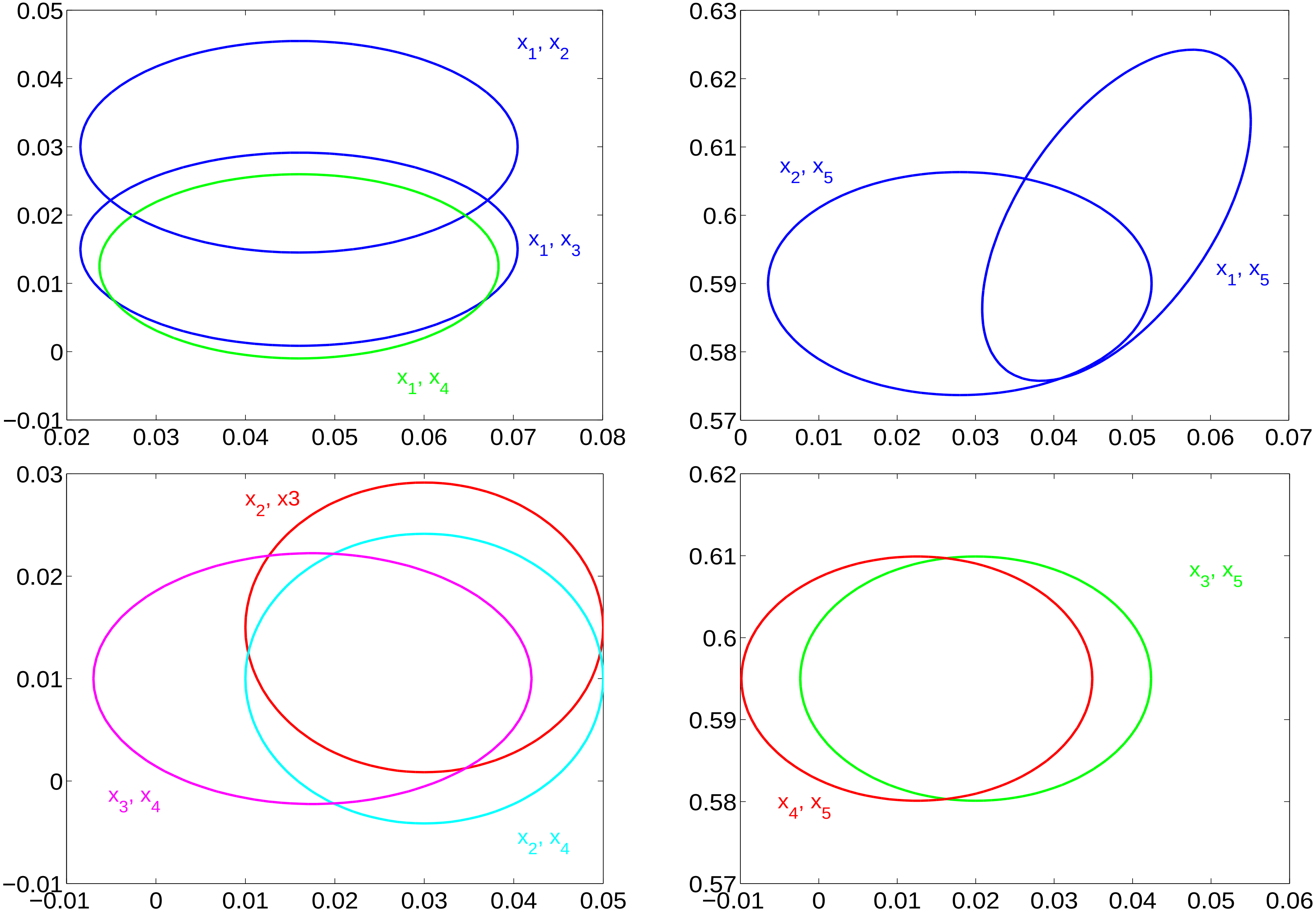
$$\boxed{\begin{aligned}
\dot{x}_0 &= -x_0 + (1 - x_3) Da \exp\left(\frac{-F}{y^2}\right) \\
\dot{x}_1 &= -x_1 + y x_0 \\
\dot{x}_2 &= -x_2 + y x_1 \\
\dot{x}_3 &= -x_3 + y x_2 \\
\dot{y} &= \frac{1 - y - (\alpha - y) y x_2}{1 - x_3} + \frac{u}{1 - x_3}
\end{aligned}}$$

  - ◇ Unstable equilibrium point surrounded by stable limit cycle.
  - ◇ Control objective:
    - ▷ Stabilization at unstable equilibrium point.
    - ▷ Input constraints: $u \in [-1, 1]$.

- Bounded controller: designed using normal form.

- Predictive controller: linear prediction model with stability constraints.

PROJECTIONS OF STABILITY REGION



- **State–space description:**

$$\begin{aligned}
\dot{x}_0 &= -x_0 + (1 - x_3) Dae^{\frac{-F}{y^2}} \\
\dot{x}_1 &= -x_1 + y x_0 \\
\dot{x}_2 &= -x_2 + y x_1 \\
\dot{x}_3 &= -x_3 + y x_2 \\
\dot{y} &= \frac{1 - y - (\alpha - y) y x_2}{1 - x_3} + \frac{u}{1 - x_3}
\end{aligned}$$

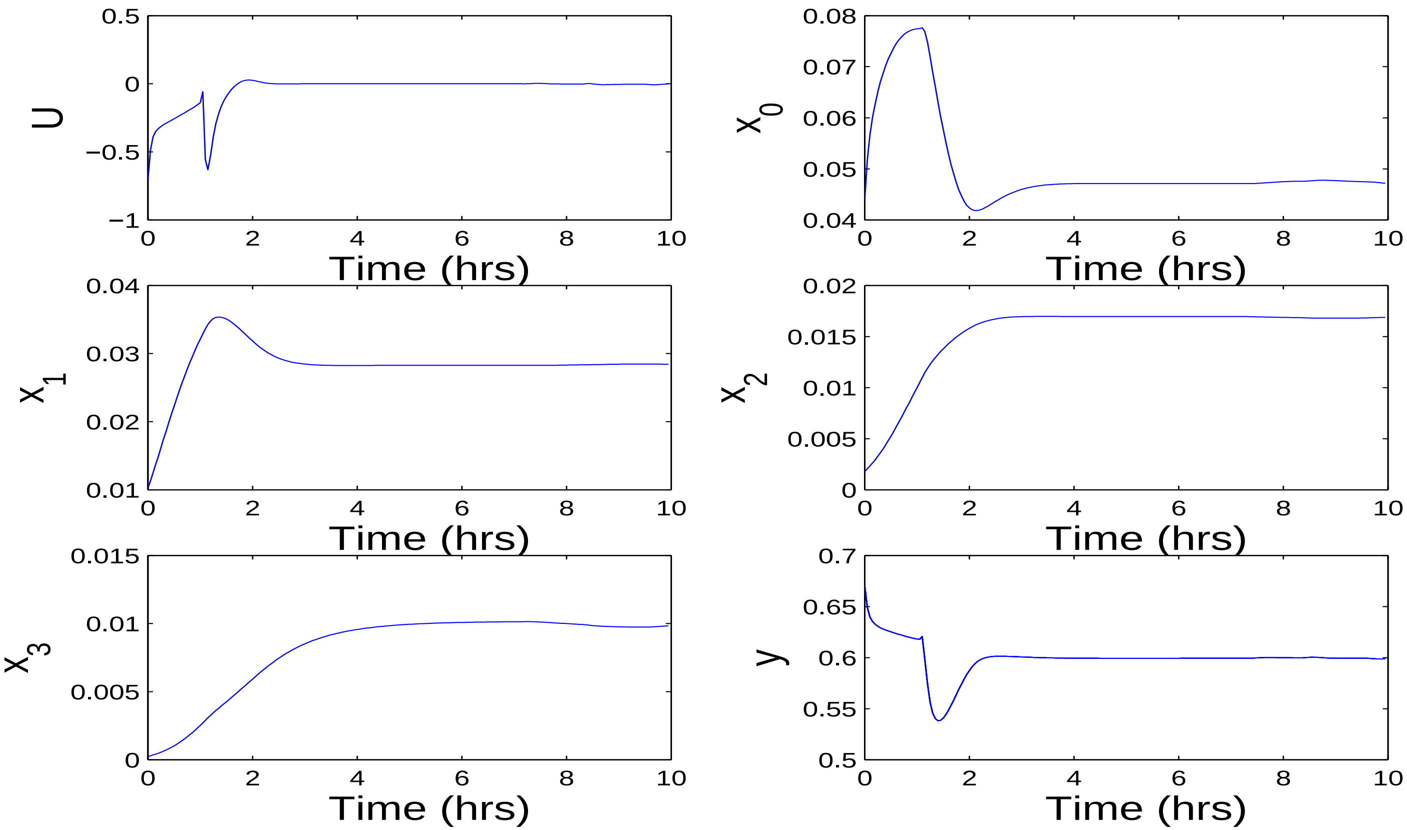
  - ◇ Unstable equilibrium point surrounded by limit cycle
  - ◇ Input constraints: $u \in [-1, 1]$

- **Bounded controller:**
  - ◇ Normal form representation:

$$\boxed{\begin{aligned}
\dot{\xi} &= A\xi + bl(\xi, \eta) + b\alpha(\xi, \eta)u \\
\dot{\eta} &= \Psi(\xi, \eta)
\end{aligned}}$$

CLOSED-LOOP SIMULATION RESULTS

"Stability-based switching"

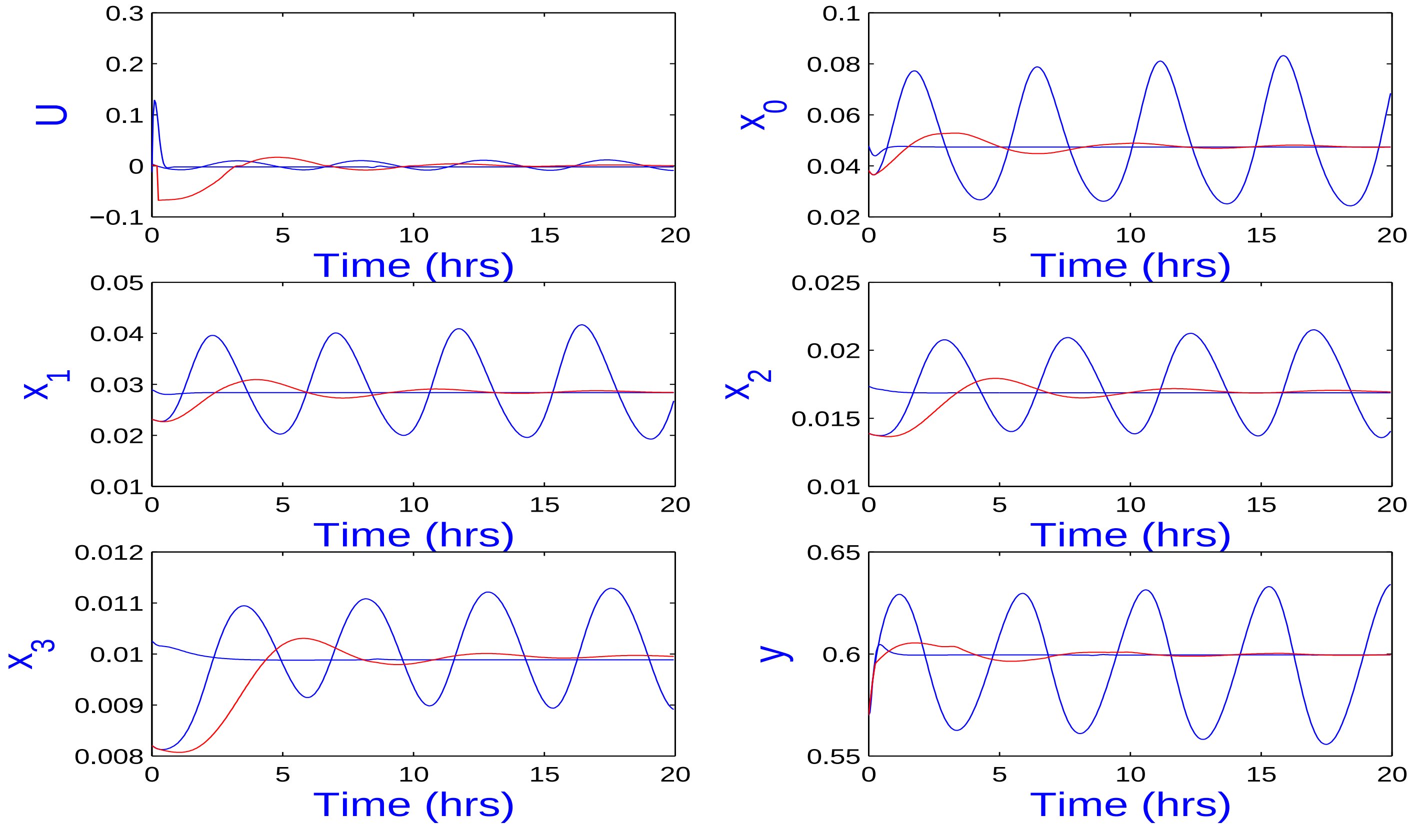


◇ Input & state profiles

◇ $x(0) = [0.044\ 0.01\ 0.022\ 0.002\ 0.67\ ]^T \in \Omega_{system}(u_{max})$

◇ MPC with $T = 0.25$, switching ($t = 1$), $J = 3.4259$

CLOSED-LOOP SIMULATION RESULTS

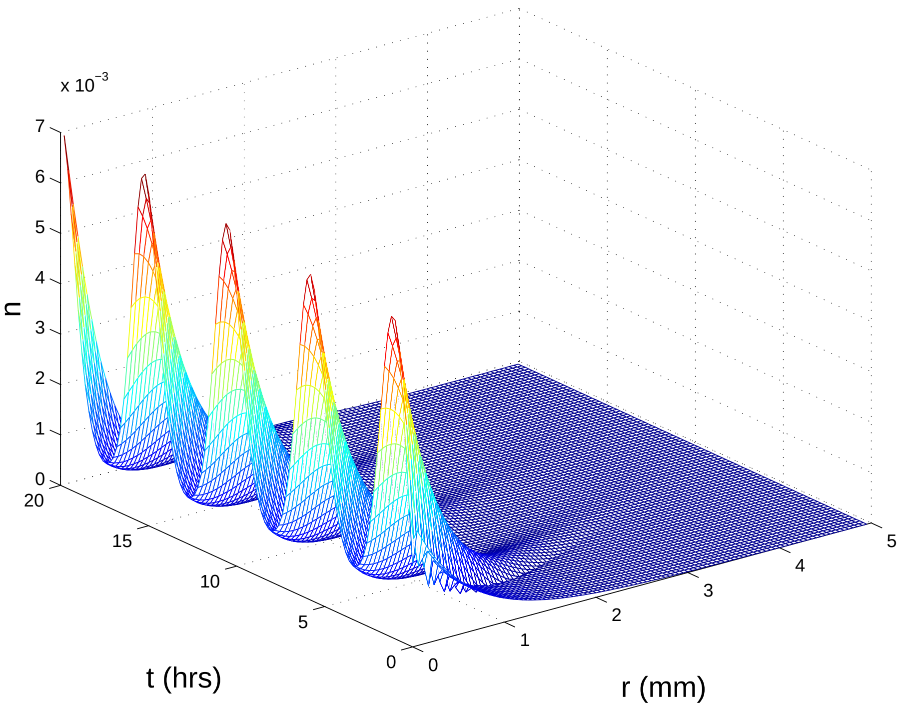


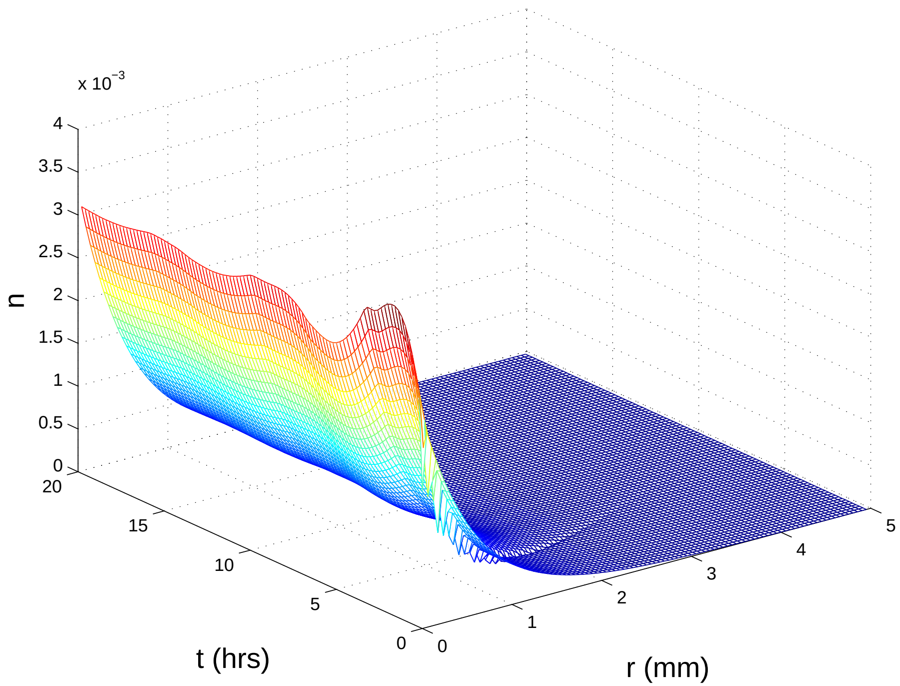
- ◇ $x_1(0)$: MPC with $T = 0.25$ feasible
- ◇ $x_2(0)$: MPC with $T = 0.25$ (no terminal constraints)
- ◇ $x_2(0)$: switching to bounded controller

CLOSED-LOOP SIMULATION RESULTS

Evolution of Crystal Size Distribution

- Closed loop simulation results of MPC with $T = 0.25$ (no terminal constraints)(left figure).
- Closed loop simulation results of Bounded controller(right figure).



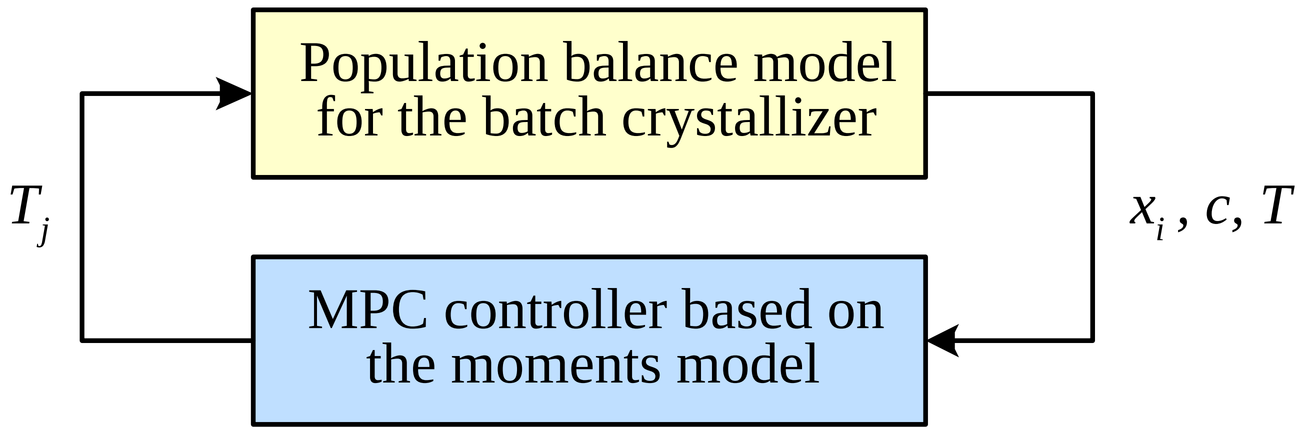


APPLICATION TO A SEEDED BATCH CRYSTALLIZER

- **Population balance model:**

$$\boxed{\begin{aligned}\frac{\partial n}{\partial t} &= -G(t)\frac{\partial n}{\partial r}\\ \frac{dc}{dt} &= -3\rho k_v G(t) x_2\\ \frac{dT}{dt} &= -\frac{UA}{MC_p}(T-T_j) - 3\frac{\Delta H}{C_p}\rho k_v G(t) x_2\end{aligned}}$$

- **Model predictive control loop structure:**



APPLICATION TO A SEEDED BATCH CRYSTALLIZER

- **Batch crystallizer moments model:**

$$\boxed{\begin{aligned}
\dot{x}_0 &= B(t) \\
\dot{x}_1 &= G(t)x_0 \\
\dot{x}_2 &= 2G(t)x_1 \\
\dot{x}_3 &= 3G(t)x_2 \\
\dot{c} &= -3\rho k_v G(t)x_2 \\
\dot{T} &= -\frac{UA}{MC_p}(T - T_j) - 3\frac{\Delta H}{C_p}\rho k_v G(t)x_2
\end{aligned}}$$

- **Manipulated variables**
  - ◇ Solute concentration
  - ◇ Heating/Cooling
- **Measured output variables**
  - ◇ Solute concentration
  - ◇ Crystal size distribution
- **Controlled output variables**
  - ◇ Shaping crystal size distribution

APPLICATION TO A SEEDED BATCH CRYSTALLIZER

- **Optimization problem:**

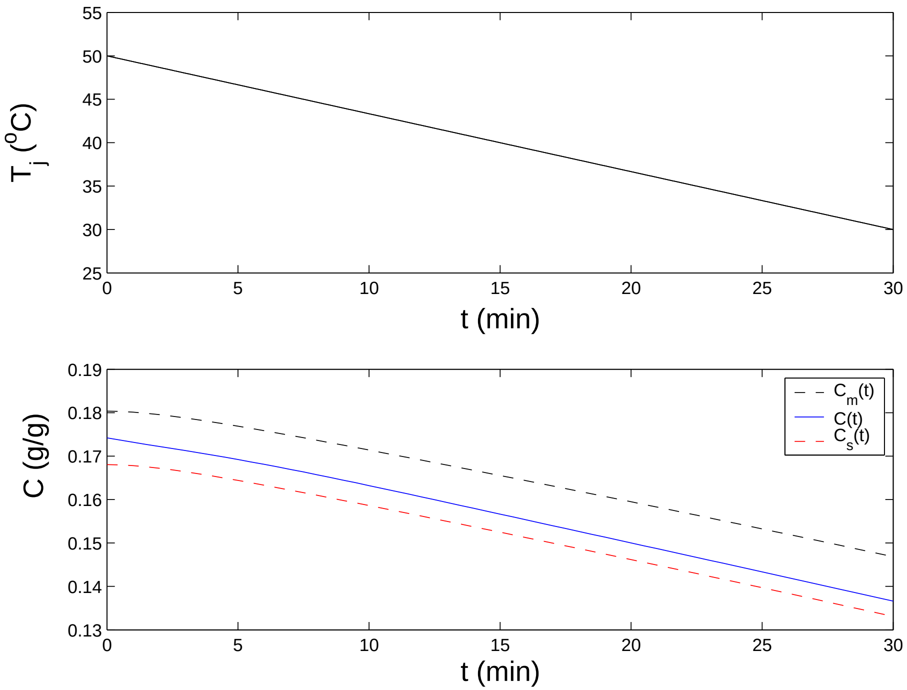
$$\boxed{\begin{array}{ll} \max & \dfrac{x_3}{x_0} \\ s.t. & T_{jmin} \leq T_j \leq T_{jmax} \\ & c_s \leq c \leq c_m \end{array}}$$

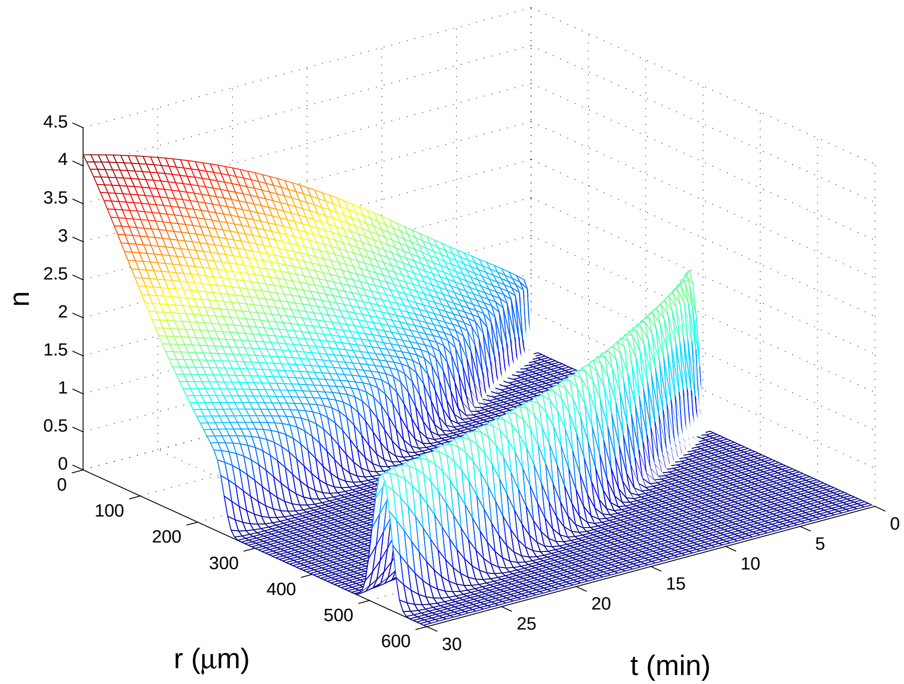
x_3	:	the third-order moment of the moments model, total volume of crystals.
x_0	:	the zero-order moment of the moments model, total number of crystals.
T_{jmin}	:	the lower bound of the jacket temperature.
T_{jmax}	:	the upper bound of the jacket temperature.
c_s	:	the saturation concentration at certain reactor temperature.
c_m	:	the metastable concentration at certain reactor temperature.

APPLICATION TO A SEEDED BATCH CRYSTALLIZER

Open Loop Simulation Results

- Open loop simulation results with linear cooling strategy. Results include the evolution of crystal size distribution(right figure), and the trajectories of the jacket temperature and the reactor concentration(left figure).
- Average crystal volume of the final product is $6.84 \times 10^7 \mu m^3$.

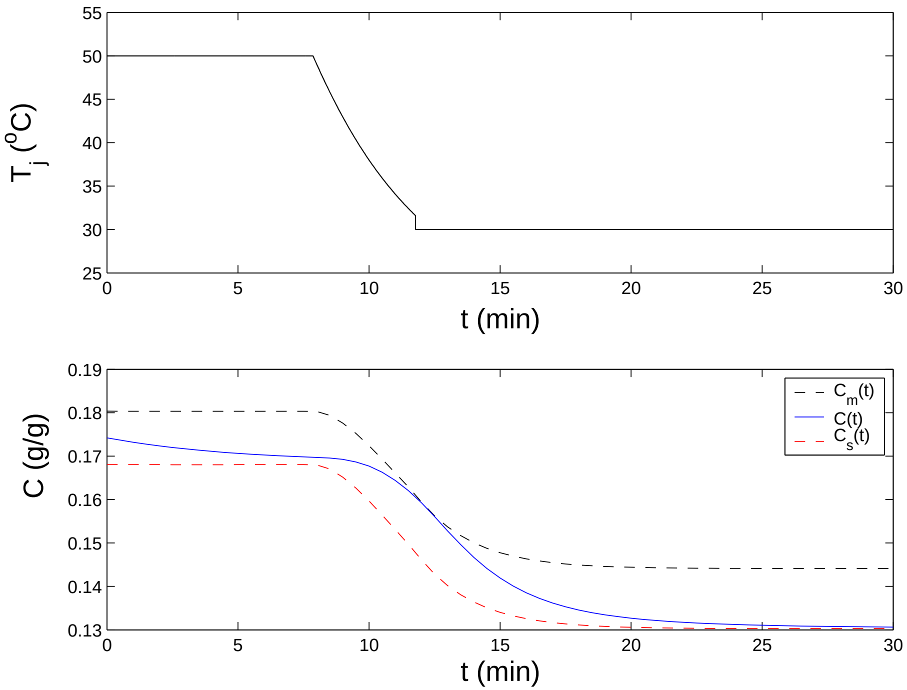


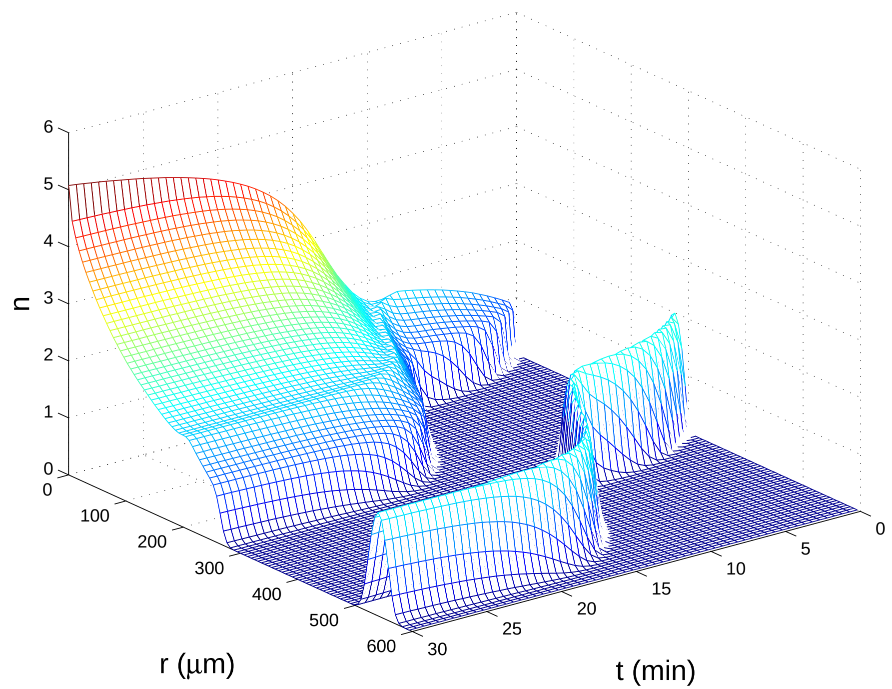


APPLICATION TO A SEEDED BATCH CRYSTALLIZER

Closed Loop Simulation Results

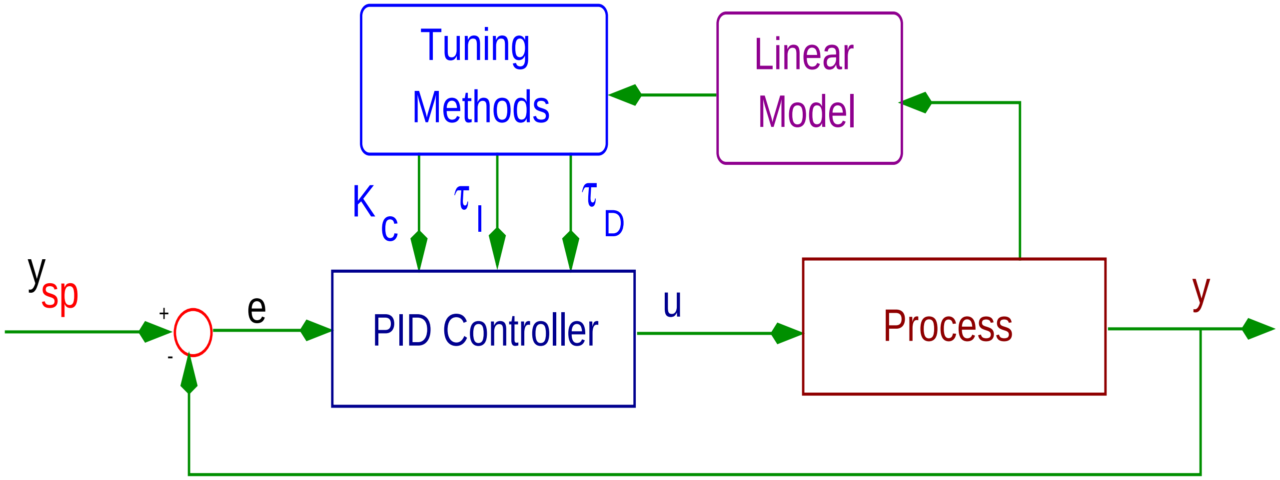
- Closed loop simulation results with MPC. Results include the evolution of crystal size distribution(right figure), and the trajectories of the jacket temperature and the reactor concentration(left figure).
- Average crystal volume of the final product is $7.58 \times 10^7 \mu m^3$.





TUNING CLASSICAL CONTROLLERS USING NONLINEAR CONTROL THEORY: PROCESS CONTROL PRACTICE

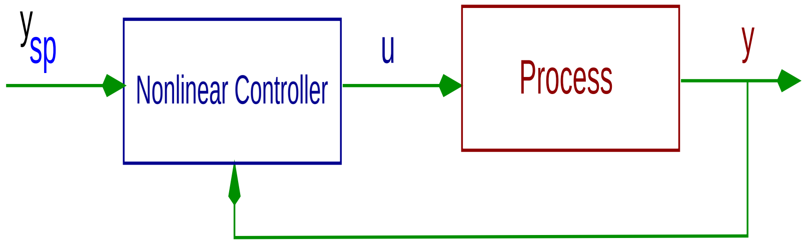
- Proportional Integral Derivative (PID) controllers:



- "Easy" to use and implement:
  - ◇ Tuning rules based on linear process models.
- Do not account for
  - ◇ Process nonlinearities, uncertainties, constraints etc.
- Extensive retuning/poor performance.

TUNING CLASSICAL CONTROLLERS USING NONLINEAR CONTROL THEORY: NONLINEAR CONTROL THEORY

- Nonlinear controllers:



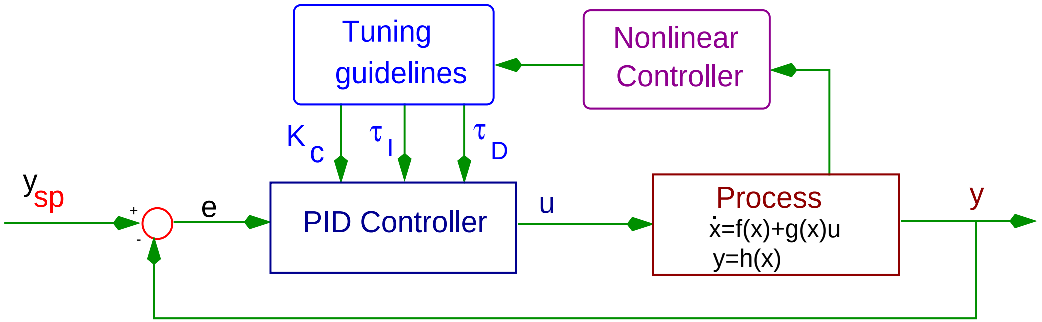
  - ◇ Handle process uncertainties/time delays/state estimation/...
  - ◇ Provide rigorous results and analysis.
  - ◇ Require better understanding of the process (detailed models).
  - ◇ Implementation requires redesign of existing control hardware.

- Gap between
  - ▷ Nonlinear control theory tools.
  - ▷ Process control practice (K_c, τ_i, τ_d).

Use/develop nonlinear control tools for PID controller tuning

TUNING GUIDELINES

- Tuning framework



◇ Design a nonlinear controller that accounts for the complex process dynamics.

◇ Compute, but not implement, the control action as prescribed by the nonlinear controller.

◇ Set up and solve an optimization problem:

▷ The objective function 'measures' the difference between the control action of the PID and the nonlinear controller.

▷ The decision variables are the PID controller parameters.

ESTIMATION AND CONTROL OF SIZE DISTRIBUTION IN AEROSOL PROCESSES

- Aerosol processes are widely used for the production of ceramic powders, such as, TiO_2, SiO_2 and other nano-/micron-sized particles.
- Mechanism of production and growth:

$$\begin{array}{cl} \text{Birth of monomers by gas-phase chemical reaction} & \\ \Downarrow & \text{condensation, aggregation of monomers} \\ \text{Nucleation of aerosol particles} & \\ \Downarrow & \text{coagulation} \\ \text{Nano-/micron- sized particles} & \end{array}$$

- Population balances models (PBMs): Natural modeling framework.
  - ⋄ Main features: nonlinear and distributed nature.

AEROSOL PROCESS MODEL

Particulate phase

- Population balance equation:

$$\frac{\partial n}{\partial t} + \frac{\partial (G(\bar{x}, v)n)}{\partial v} - I(v^*)\delta(v - v^*)$$

$$= \frac{1}{2}\int_0^v \beta(v-\bar{v}, \bar{v}, \bar{x}) n(v-\bar{v}, t) n(\bar{v}, t) d\bar{v}$$

$$-n(v,t)\int_0^\infty \beta(v, \bar{v}, \bar{x}) n(\bar{v}, t) d\bar{v}$$

$n(v,t)$	:	aerosol size distribution function
t	:	time
v	:	particle volume
$G(\bar{x}, v)$	:	growth function
$I(v^*)$	:	nucleation rate
$\beta(v-\bar{v}, \bar{v}, \bar{x})$	:	coagulation coefficient

AEROSOL PROCESS MODEL

Continuous phase

- Mass and energy balances:

$$\frac{d\bar{x}}{dt} = +\bar{f}(\bar{x}) + \bar{g}(\bar{x})u(t) + \tilde{A}\int_0^\infty a(\eta, v, x)dv$$

$\bar{x}(t)$	:	n-dimensional vector of continuous phase variables (e.g., temperature, concentrations)
$\bar{f}(\bar{x}), \bar{g}(\bar{x}), a(\eta, v, x)$	:	nonlinear vector functions
$\bar{A}, \tilde{A}$	:	constant matrices
$\tilde{A}\int_0^\infty a(\eta, v, \bar{x})dv$	:	mass/heat transfer from the continuous to the particle phase
$u(t)$	:	manipulated variable

- System of nonlinear first-order ordinary differential equations.

METHODOLOGICAL FRAMEWORK FOR ESTIMATION AND CONTROL

- Aerosol process model.

$$\frac{\partial n}{\partial t} + \frac{\partial (G(\bar{x}, v)n)}{\partial v} - I(v^*)\delta(v - v^*)$$
$$= \frac{1}{2}\int_0^v \beta(v - \bar{v}, \bar{v}, \bar{x})n(v - \bar{v}, t)n(\bar{v}, t)d\bar{v} - n(v, t)\int_0^\infty \beta(v, \bar{v}, \bar{x})n(\bar{v}, t)d\bar{v}$$

$$\frac{d\bar{x}}{dt} = \bar{f}(\bar{x}) + \bar{g}(\bar{x})u(t) + \tilde{A}\int_0^\infty a(\eta, v, \bar{x})dv$$

- Methodology for estimation and controller design.
  - ◇ Nonlinear model reduction of population balance equations.
    - ▷ Lognormal aerosol size distribution.
    - ▷ Method of moments.
  - ◇ Nonlinear output feedback controller design.
  - ◇ Validation through implementation on the sectional model.

LOGNORMAL AEROSOL SIZE DISTRIBUTION

- Many aerosol size distributions can be adequately modeled by lognormal functions (Pratsinis, JCIS, 1988).

$$n(v,t) = \frac{1}{3\sqrt{2\pi} ln\sigma} exp\left(-\frac{ln^2(v/v_g)}{18 ln^2\sigma}\right)\frac{1}{v}$$

v_g : geometric average particle volume

$$v_g = \frac{M_1^2}{M_0^{\frac{3}{2}} M_2^{\frac{1}{2}}}$$

σ : standard deviation

$$ln^2\sigma = \frac{1}{9} ln\left(\frac{M_0 M_2}{M_1^2}\right)$$

M_0, M_1 and M_2 are the three leading volume weighted moments, and:

$$M_k(t) = \int_0^\infty v^k n(v,t)dv = M_0 v_g^k exp\left(\frac{9}{2}k^2 ln^2\sigma\right)$$

- Lognormal aerosols can be adequately described by moment models.

DERIVATION OF MOMENT MODEL

$$\frac{\partial n}{\partial t} + \frac{\partial (G(\bar{x}, v)n)}{\partial v} - I(v^*)\delta(v - v^*)$$

$$= \frac{1}{2}\int_0^v \beta(v - \bar{v}, \bar{v}, \bar{x}) n(v - \bar{v}, t) n(\bar{v}, t) d\bar{v}$$

$$- n(v, t)\int_0^\infty \beta(v, \bar{v}, \bar{x}) n(\bar{v}, t) d\bar{v}$$

- Multiplication with v^k and integration over all particle size.
- Approximation of $n(v, t)$ by a lognormal function.
- Aerosol dynamics over the entire particle spectrum is described by using harmonic means of dimensionless coefficients in free-molecular and continuum regions.

MOMENT MODEL

- Zeroth moment (aerosol concentration):

$$\frac{dN}{d\theta} = I' - \xi N^2$$

- First moment (aerosol volume):

$$\frac{dV}{d\theta} = I'k^* + \eta(S-1)N$$

- Second moment:

$$\frac{dV_2}{d\theta} = I'{k^*}^2 + 2\epsilon(S-1)V + 2\zeta V^2$$

ξ, ζ : dimensionless coagulation coefficients

$$\frac{1}{\xi} = \frac{1}{\xi_{FM}} + \frac{1}{\xi_C}, \quad \frac{1}{\zeta} = \frac{1}{\zeta_{FM}} + \frac{1}{\zeta_C}$$

ϵ, η : dimensionless condensation coefficients

$$\frac{1}{\epsilon} = \frac{1}{\epsilon_{FM}} + \frac{1}{\epsilon_C} \quad , \quad \frac{1}{\eta} = \frac{1}{\eta_{FM}} + \frac{1}{\eta_C}$$

MODEL USED FOR ESTIMATOR AND CONTROLLER DESIGN

- Moment model:

$$\begin{aligned}\frac{dN}{d\theta} &= I' - \xi N^2 \\ \frac{dV}{d\theta} &= I'k^* + \eta(S-1)N \\ \frac{dV_2}{d\theta} &= I'{k^*}^2 + 2\epsilon(S-1)V + 2\zeta V^2\end{aligned}$$

- Material and energy balances (continuous phase):

$$\frac{d\bar{x}}{dt} = \bar{f}(\bar{x}) + \bar{g}(\bar{x})u(t) + \tilde{A}\int_0^\infty a(\eta, v, \bar{x})dv$$

- Introducing $x = [N \ V \ V_2 \ \bar{x}]^T$:

$$\begin{aligned}\frac{dx}{dt} &= f(x) + g(x)u \\ y &= h(x)\end{aligned}$$

y: controlled output variable.

NONLINEAR ESTIMATOR / CONTROLLER DESIGN

$$\begin{aligned}\frac{dx}{dt} &= f(x) + g(x)u \\ y &= h(x)\end{aligned}$$

- **Feedback linearization:**
  - Controller synthesis formula

$$u = \frac{1}{L_g L_f^{r-1} h(x)} \left(v - L_f^r h(x) - \sum_{k=1}^{r} \beta_k L_f^{r-k} h(x) \right)$$

Lie derivative notation: $L_f h(x) = \dfrac{\partial h}{\partial x} f(x)$.

  - Input/Output Dynamics

$$\frac{d^r y}{dt} + \beta_1 \frac{d^{r-1} y}{dt} + \cdots + \beta_{r-1} \frac{dy}{dt} + \beta_r y = v$$

$\beta_1, \cdots, \beta_r$ are tuning parameters (time constants).

- **Nonlinear state estimator design:**
  - Nonlinear Luenberger-type state estimator.

$$\frac{d\eta}{dt} = f(\eta) + g(\eta)u + L(y - h(\eta))$$

  - L: observer gain.

APPLICATION TO A BATCH AEROSOL REACTOR

- Batch aerosol reactor: $A + B \rightarrow C$.
- Chemical reaction, nucleation, condensation and coagulation.
- Sectional model:

$$\frac{dN_1}{dt} = I(v^*)\theta(v_0 < v^* < v_1) - \frac{1}{2}{}^3\bar{\beta}_{1,1}N_1^2 - N_1\sum_{i=2}^{m}{}^4\bar{\beta}_{i,1}N_i - \xi_1 N_1,$$

$$\begin{aligned}\frac{dN_l}{dt} &= I(v^*)\theta(v_{l-1} < v^* < v_l) + \frac{1}{2}\sum_{i=1}^{l-1}\sum_{j=1}^{l-1}{}^1\bar{\beta}_{i,j,l}N_iN_j \\ &\quad -N_l\sum_{i=1}^{l-1}{}^2\bar{\beta}_{i,l}N_i - \frac{1}{2}{}^3\bar{\beta}_{l,l}N_l^2 \\ &\qquad -N_l\sum_{i=l+1}^{m}{}^4\bar{\beta}_{i,l}N_i + \xi_{l-1}N_{l-1} - \xi_l N_l, \qquad 2 \leq\end{aligned}$$

- Sectional model(cont.):

$$\begin{aligned}
\frac{dN_m}{dt} &= I(v^*)\theta(v_{m-1} < v^* < v_m) + \frac{1}{2}\sum_{i=1}^{m-1}\sum_{j=1}^{m-1}{}^1\bar{\beta}_{i,j,m}N_iN_j \\
&\quad -N_l\sum_{i=1}^{m-1}{}^2\bar{\beta}_{i,m}N_i \\
&\quad -\frac{1}{2}{}^3\bar{\beta}_{m,m}N_m^2 + \xi_{m-1}N_{m-1} \\
\frac{dn_0}{dt} &= k_rC_1C_2N_{av} - Ik^* - \\
&\quad omega\sum_{l=1}^{m}\frac{N_l}{(v_l - v_{l-1})}\int_{v_{l-1}}^{v_l} v^{\frac{1}{3}}\frac{1+Kn}{1+1.71Kn+1.333Kn^2}dv \\
\frac{dC_1}{dt} &= -k_rC_1C_2 \\
\frac{dC_2}{dt} &= -k_rC_1C_2 \\
\frac{dT}{dt} &= (k_rC_1C_2\Delta H_r + 4UD_T^{-1}(T_w - T))C_{pv}^{-1}
\end{aligned}$$

MOMENT MODEL / CONTROL PROBLEM

- Moment model.

$$\begin{aligned}
\frac{dN}{dt} &= I' - \xi N^2 \\
\frac{dV}{dt} &= I'k^* + \eta(S-1)N \\
\frac{dV_2}{dt} &= I'k^{*2} + 2\epsilon(S-1)V + 2\zeta V^2 \\
\frac{dS}{dt} &= C\bar{C}_1\bar{C}_2 - I'k^* - \eta(S-1)N \\
\frac{d\bar{C}_1}{dt} &= -A_1\bar{C}_1\bar{C}_2 \\
\frac{d\bar{C}_2}{dt} &= -A_2\bar{C}_1\bar{C}_2 \\
\frac{d\bar{T}}{dt} &= B\bar{C}_1\bar{C}_2\bar{T} + E\bar{T}(\bar{T}_w - \bar{T})
\end{aligned}$$

- Control problem
  - ◇ Controlled output: v_g at the end of the batch.
  - ◇ Manipulated input: T_w.

ESTIMATION AND CONTROL OF SIZE DISTRIBUTION IN AEROSOL PROCESSES

(Kalani and Christofides, AIChE J., 2002)

- Spatially homogeneous aerosol processes described by population balances.

- General framework for nonlinear state estimation and feedback control.

  ◇ Sectional and moment approximations.

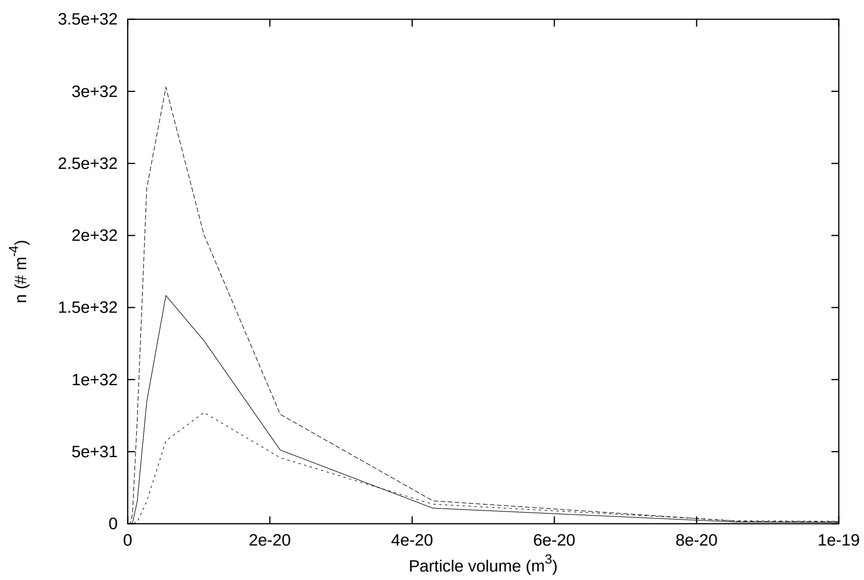
  ◇ Estimator and controller design based on the moment models.

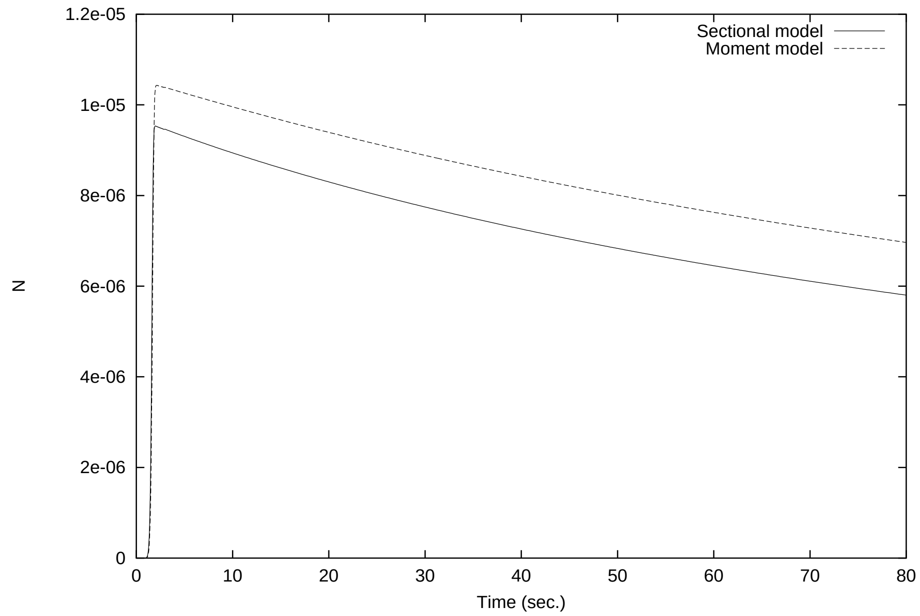
  ◇ Validation through implementation on the sectional model.

- Application to an aerosol process with nucleation, condensation and coagulation.

OPEN-LOOP SIMULATION RESULTS

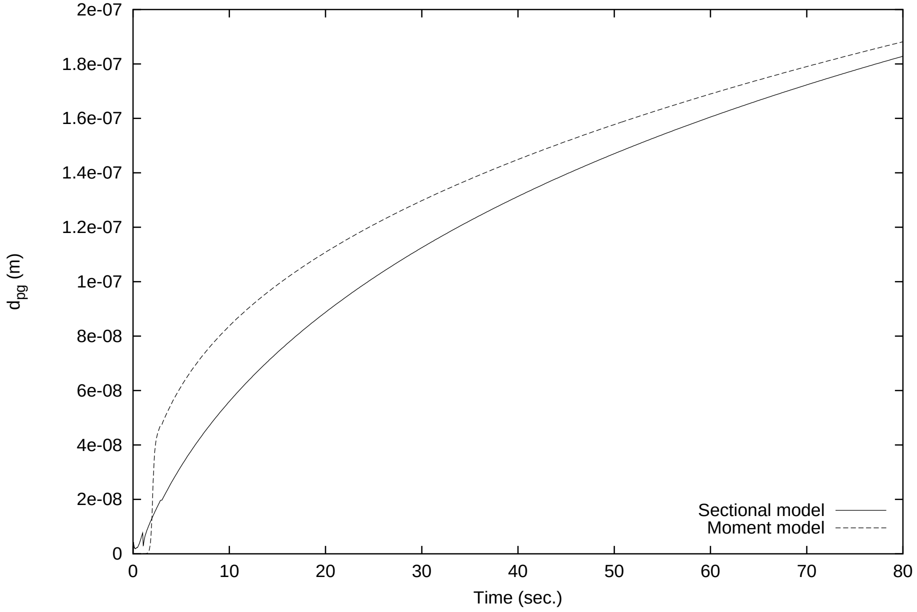
- Profiles of N computed by the sectional (solid line) and moment (dashed line) models(left figure).
- Profiles of aerosol size distribution function at $t = 80$ sec(right figure).

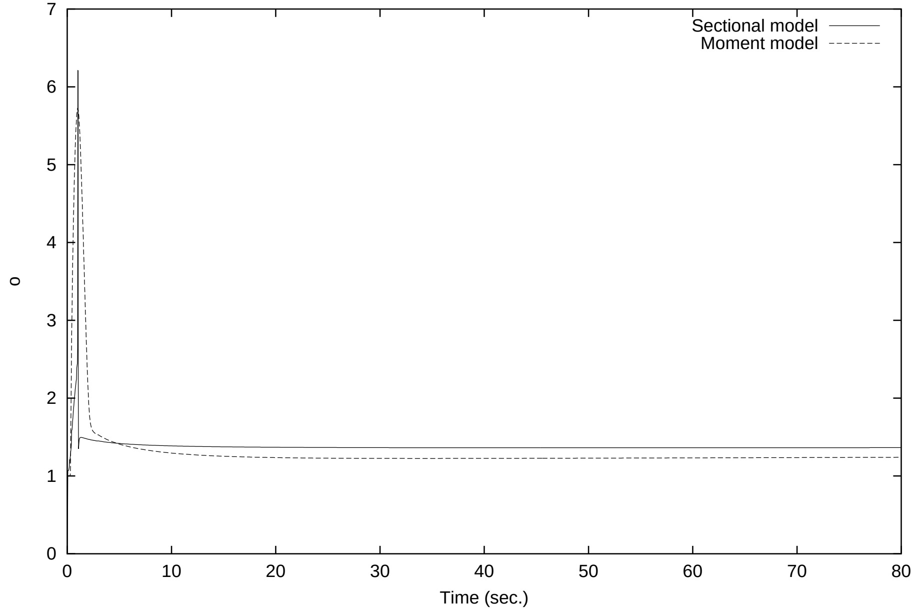




OPEN-LOOP SIMULATION RESULTS

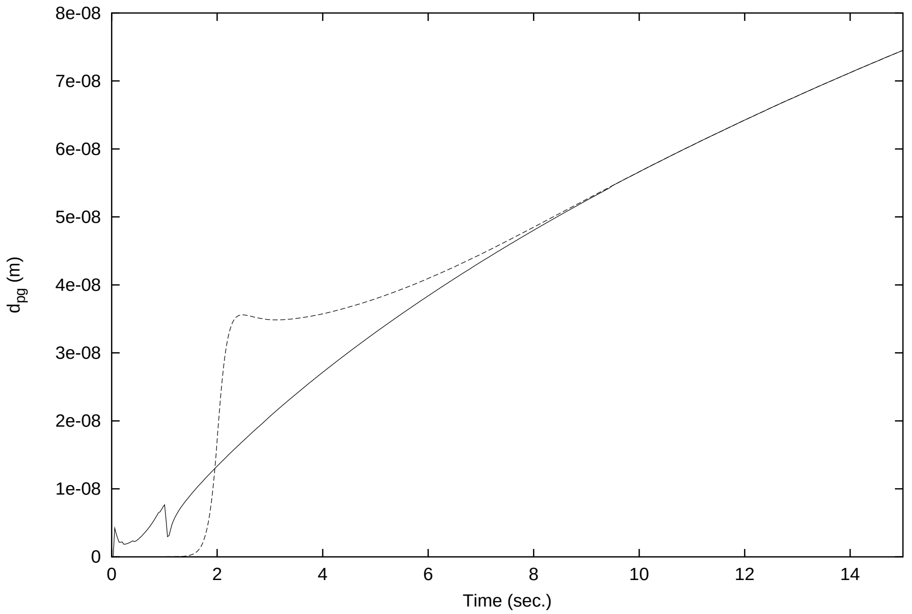
- Profiles of d_{pg} computed by the sectional (solid line) and moment (dashed line) models(left figure).
- Profiles of σ computed by the sectional (solid line) and moment (dashed line) models(right figure).

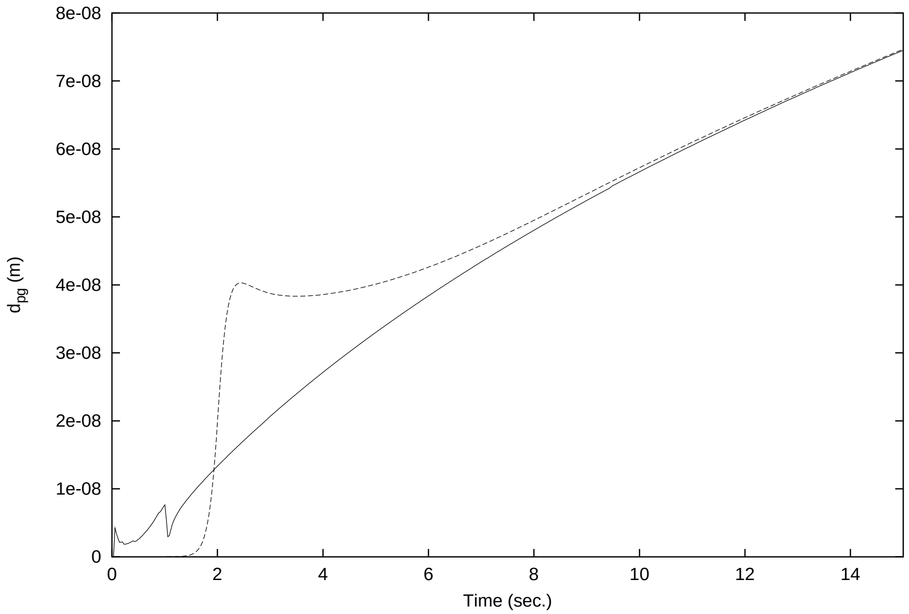




OPEN-LOOP STATE ESTIMATION RESULTS

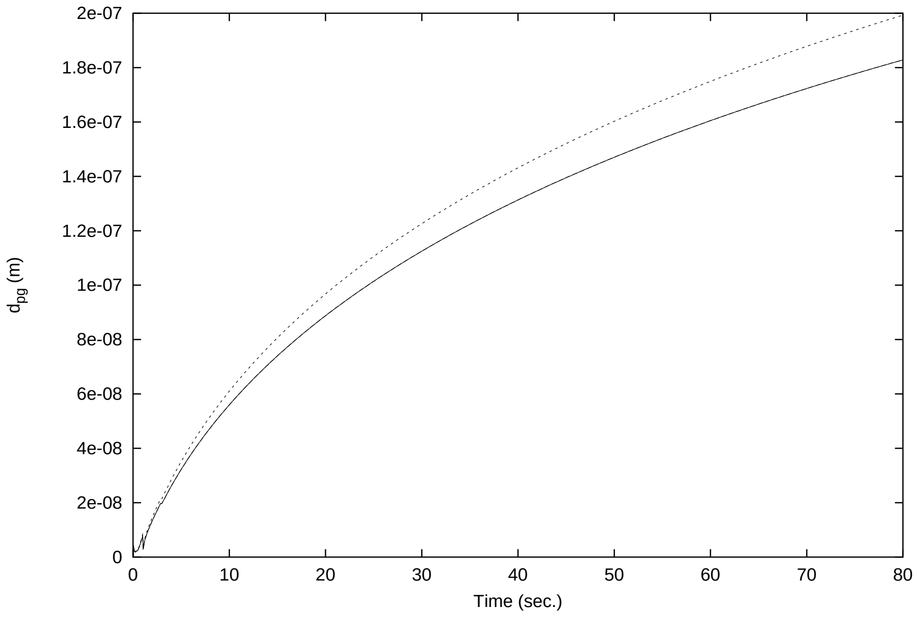
- Profiles of d_{pg} computed by the sectional model (solid line) and the state estimator (dashed line) under nominal conditions(left figure).
- Profiles of d_{pg} computed by the sectional model (solid line) and the state estimator (dashed line) under parametric uncertainty in μ, D_f, v_0(right figure).

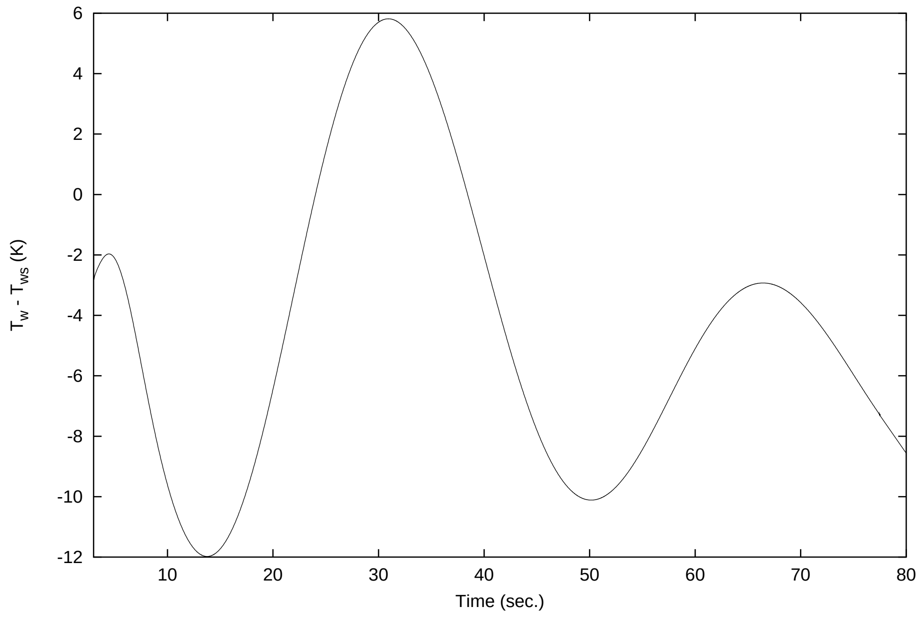




CLOSED-LOOP SIMULATION RESULTS

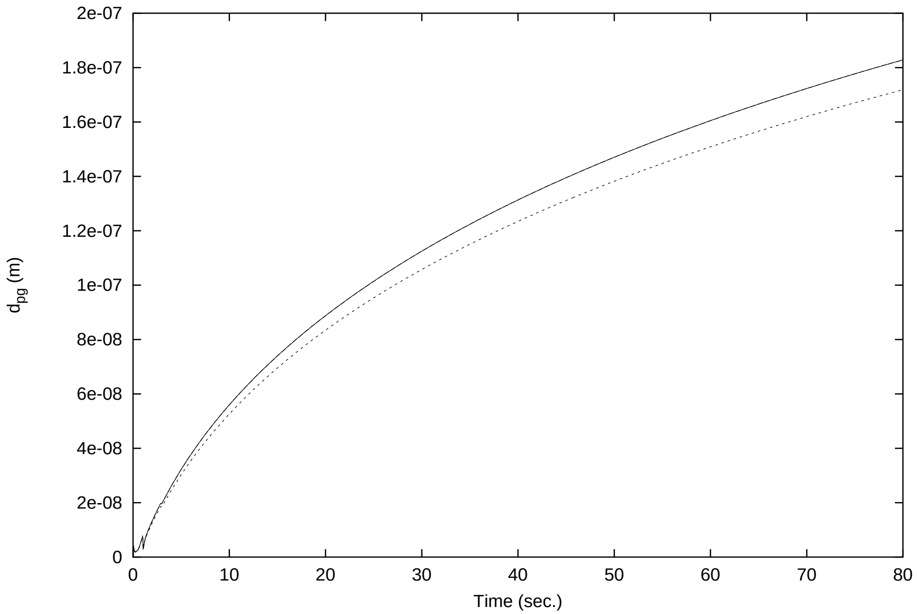
- Open-loop profile (dashed line) and closed-loop profile (solid line) of d_{pg} under uncertainty in the reaction rate constant(left figure).
- Manipulated input profile(right figure).

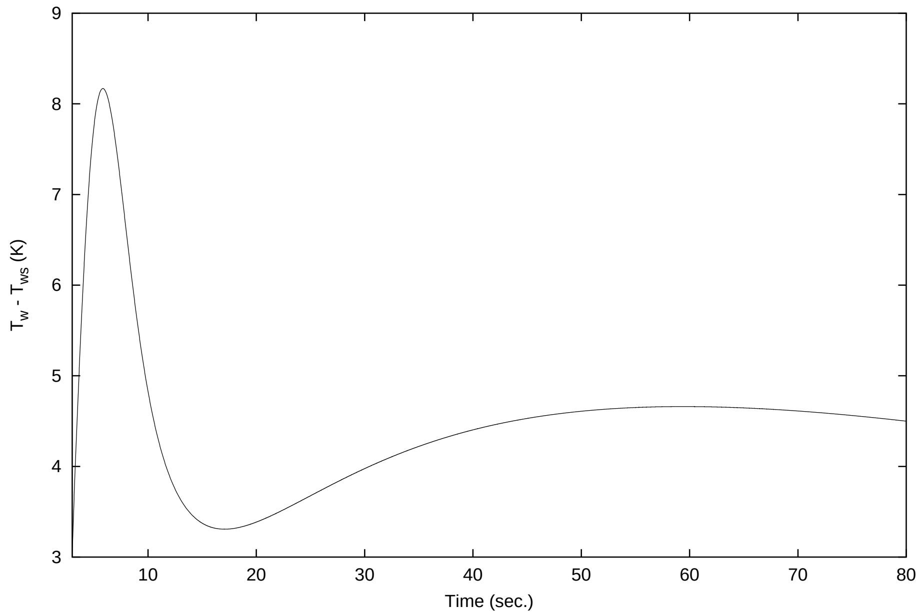




CLOSED-LOOP SIMULATION RESULTS

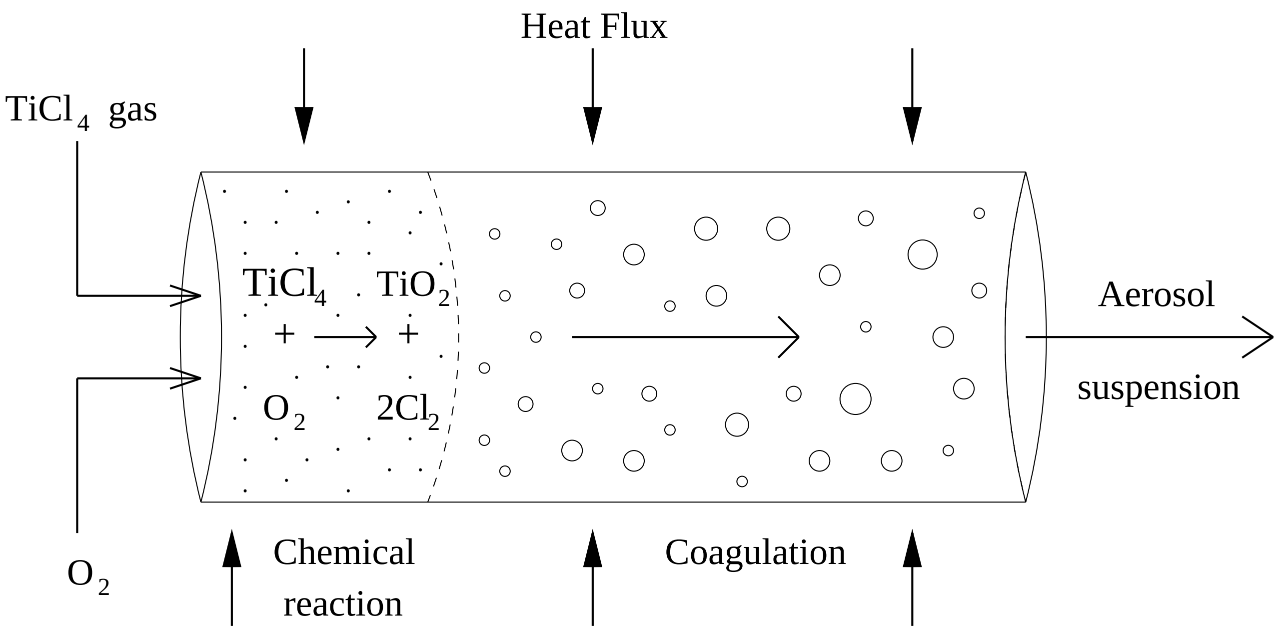
- Open-loop profile (dashed line) and closed-loop profile (solid line) of d_{pg} under uncertainty in the saturation pressure(left figure).
- Manipulated input profile(right figure).





SPATIALLY INHOMOGENEOUS AEROSOL PROCESSES

- Spatially inhomogeneous aerosol processes described by population balances.
  - ◇ A typical aerosol process.



- General framework for the synthesis of nonlinear practically-implementable controllers (Kalani and Christofides, CES, 1999a).
- Application to a titania aerosol reactor (Kalani and Christofides, AST, 2000).

AEROSOL PROCESS MODEL

Particulate phase

- Population balance equation:

$$\frac{\partial n}{\partial t} + v_z \frac{\partial n}{\partial z} + \frac{\partial (G(\bar{x}, v, z) n)}{\partial v} - I(v^*)\delta(v - v^*)$$
$$= \frac{1}{2}\int_0^v \beta(v - \bar{v}, \bar{v}, \bar{x}) n(v - \bar{v}, t) n(\bar{v}, t) d\bar{v}$$
$$- n(v, t) \int_0^\infty \beta(v, \bar{v}, \bar{x}) n(\bar{v}, t) d\bar{v}$$

$n(v, z, t)$	:	aerosol size distribution function
t	:	time
z	:	spatial coordinate
v	:	particle volume
v_z	:	fluid velocity
$G(\bar{x}, v, z)$	:	growth function
$I(v^*)$	:	nucleation rate
$\beta(v - \bar{v}, \bar{v}, \bar{x})$	:	coagulation coefficient

AEROSOL PROCESS MODEL

Continuous phase

- Mass and energy balances:

$$\frac{\partial \bar{x}}{\partial t} = \bar{A}\frac{\partial \bar{x}}{\partial z} + \bar{f}(\bar{x}) + \bar{g}(\bar{x})u(z,t) + \tilde{A}\int_0^\infty a(\eta, v, x)dv$$

$\bar{x}(z,t)$	:	n-dimensional vector of continuous phase variables (e.g.
$\bar{f}(\bar{x}), \bar{g}(\bar{x}), a(\eta, v, x)$	:	nonlinear vector functions
$\bar{A}, \tilde{A}$	:	constant matrices
$\tilde{A}\int_0^\infty a(\eta, v, \bar{x})dv$	:	mass/heat transfer from the continuous to the particle
$u(z,t)$	:	manipulated variable

- Convection-reaction equation: System of first-order hyperbolic PDEs.

METHODOLOGICAL FRAMEWORK FOR CONTROL

- Aerosol process model.

$$\frac{\partial n}{\partial t} + v_z \frac{\partial n}{\partial z} + \frac{\partial (G(\bar{x}, v, z)n)}{\partial v} - I(v^*)\delta(v - v^*)$$
$$= \frac{1}{2}\int_0^v \beta(v-\bar{v}, \bar{v}, \bar{x}) n(v-\bar{v}, t) n(\bar{v}, t) d\bar{v} - n(v,t)\int_0^\infty \beta(v, \bar{v}, \bar{x}) n(\bar{v}, t) d\bar{v}$$

$$\frac{\partial \bar{x}}{\partial t} = \bar{A}\frac{\partial \bar{x}}{\partial z} + \bar{f}(\bar{x}) + \bar{g}(\bar{x}) b(z) u(z,t) + \tilde{A}\int_0^\infty a(\eta, v, \bar{x}) dv$$

- Methodology for controller design.
  - ◇ Nonlinear model reduction of population balance equations.
    - ▷ Lognormal aerosol size distribution.
    - ▷ Method of moments.
  - ◇ Nonlinear output feedback controller design. (Christofides and Daoutidis, AIChE J., 1996)

LOGNORMAL AEROSOL SIZE DISTRIBUTION

- Many aerosol size distributions can be adequately modeled by lognormal functions (Pratsinis, JCIS, 1988).

$$n(v,t) = \frac{1}{3\sqrt{2\pi}ln\sigma} exp\left(-\frac{ln^2(v/v_g)}{18ln^2\sigma}\right)\frac{1}{v}$$

v_g : geometric average particle volume

$$v_g = \frac{M_1^2}{M_0^{\frac{3}{2}} M_2^{\frac{1}{2}}}$$

σ : standard deviation

$$ln^2\sigma = \frac{1}{9} ln\left(\frac{M_0 M_2}{M_1^2}\right)$$

M_0, M_1 and M_2 are the three leading volume weighted moments, and:

$$M_k(t) = \int_0^\infty v^k n(v,t)dv = M_0 v_g^k exp\left(\frac{9}{2}k^2 ln^2\sigma\right)$$

- Lognormal aerosols can be adequately described by moment models.

DERIVATION OF MOMENT MODEL

$$\frac{\partial n}{\partial t} + v_z \frac{\partial n}{\partial z} + \frac{\partial (G(\bar{x}, v, z) n)}{\partial v} - I(v^*)\delta(v - v^*)$$

$$= \frac{1}{2}\int_0^v \beta(v - \bar{v}, \bar{v}, \bar{x}) n(v - \bar{v}, t) n(\bar{v}, t) d\bar{v}$$

$$- n(v, t)\int_0^\infty \beta(v, \bar{v}, \bar{x}) n(\bar{v}, t) d\bar{v}$$

- Multiplication with v^k and integration over all particle size.
- Approximation of $n(v, z, t)$ by a lognormal function.
- Aerosol dynamics over the entire particle spectrum is described by using harmonic means of dimensionless coefficients in free-molecular and continuum regions.

MOMENT MODEL

- Zeroth moment (aerosol concentration):

$$\frac{\partial N}{\partial \theta} = -v_{zl}\frac{\partial N}{\partial \bar{z}} + I' - \xi N^2$$

- First moment (aerosol volume):

$$\frac{\partial V}{\partial \theta} = -v_{zl}\frac{\partial V}{\partial \bar{z}} + I'k^* + \eta(S-1)N$$

- Second moment:

$$\frac{\partial V_2}{\partial \theta} = -v_{zl}\frac{\partial V_2}{\partial \bar{z}} + I'k^{*2} + 2\epsilon(S-1)V + 2\zeta V^2$$

ξ, ζ : dimensionless coagulation coefficients

$$\frac{1}{\xi} = \frac{1}{\xi_{FM}} + \frac{1}{\xi_C}, \quad \frac{1}{\zeta} = \frac{1}{\zeta_{FM}} + \frac{1}{\zeta_C}$$

ϵ, η : dimensionless condensation coefficients

$$\frac{1}{\epsilon} = \frac{1}{\epsilon_{FM}} + \frac{1}{\epsilon_C} \quad , \quad \frac{1}{\eta} = \frac{1}{\eta_{FM}} + \frac{1}{\eta_C}$$

MODEL USED FOR ESTIMATOR AND CONTROLLER DESIGN

- Moment model:

$$\begin{aligned}
\frac{\partial N}{\partial \theta} &= -v_{zl}\frac{\partial N}{\partial \bar{z}} + I' - \xi N^2 \\
\frac{\partial V}{\partial \theta} &= -v_{zl}\frac{\partial V}{\partial \bar{z}} + I'k^* + \eta(S-1)N \\
\frac{\partial V_2}{\partial \theta} &= -v_{zl}\frac{\partial V_2}{\partial \bar{z}} + I'{k^*}^2 + 2\epsilon(S-1)V + 2\zeta V^2
\end{aligned}$$

- Material and energy balances (continuous phase):

$$\frac{\partial \bar{x}}{\partial t} = \bar{A}\frac{\partial \bar{x}}{\partial z} + \bar{f}(\bar{x}) + \bar{g}(\bar{x})u(z,t) + \tilde{A}\int_0^{\infty} a(\eta, v, \bar{x})dv$$

- Introducing $x = [N \; V \; V_2 \; \bar{x}]^T$:

$$\begin{aligned}
\frac{\partial x}{\partial t} &= A\frac{\partial x}{\partial z} + f(x) + g(x)u \\
y &= h(x)
\end{aligned}$$

y: controlled output variable.

SPECIFICATION OF THE CONTROL PROBLEM

- l : number of control actuators
- $b^i(z)$: actuator distribution function
- $\bar{y}^i = \mathcal{C}^i h(x) = \int_{z_i}^{z_{i+1}} c^i(\tilde{z}) h(x(\tilde{z},t)) d\tilde{z}$
- $c^i(z)$: depends on performance specifications

$$\frac{\partial x}{\partial t} = A \frac{\partial x}{\partial z} + f(x) + g(x) \sum_{i=1}^{l} \left(H(z - z_i) - H(z - z_{i+1}) \right) b^i(z) \bar{u}^i(t)$$

$$\bar{y}^i(t) = \mathcal{C}^i h(x) \ , \ i = 1, \cdots, l$$

CHARACTERISTIC INDEX

- Lowest order time-derivative of $\bar{y}^i$ which depends on $\bar{u}^i$.

$$
\begin{aligned}
\bar{y}^i &= \mathcal{C}^i h(x) \\
\frac{\partial \bar{y}^i}{\partial t} &= \mathcal{C}^i \left(\sum_{j=1}^{n} \frac{\partial x_j}{\partial z} L_{a_j} + L_f \right) h(x) \\
\frac{\partial^2 \bar{y}^i}{\partial t^2} &= \mathcal{C}^i \left(\sum_{j=1}^{n} \frac{\partial x_j}{\partial z} L_{a_j} + L_f \right)^2 h(x) \\
&\vdots \\
\frac{\partial^{\sigma^i} \bar{y}^i}{\partial t^{\sigma^i}} &= \mathcal{C}^i \left(\sum_{j=1}^{n} \frac{\partial x_j}{\partial z} L_{a_j} + L_f \right)^{\sigma^i} h(x) \\
&\quad + \mathcal{C}^i L_g \left(\sum_{j=1}^{n} \frac{\partial x_j}{\partial z} L_{a_j} + L_f \right)^{\sigma^i - 1} h(x) b^i(z) \bar{u}^i
\end{aligned}
$$

- Dependence on actuator distribution function
- $\sigma^1 = \sigma^2 = \cdots = \sigma^l = \sigma$

DISTRIBUTED STATE FEEDBACK CONTROL

- Systems of Quasi-linear PDEs

$$\frac{\partial x}{\partial t} = A\frac{\partial x}{\partial z} + f(x) + g(x)\sum_{i=1}^{l}\left(H(z-z_i) - H(z-z_{i+1})\right)b^i(z)\bar{u}^i(t)$$

$$\bar{y}^i(t) = \mathcal{C}^i h(x)\ ,\ i = 1, \cdots, l$$

- Distributed state feedback controller :

$$\bar{u}^i = \left[\mathcal{C}^i \gamma_\sigma L_g \left(\sum_{j=1}^{n}\frac{\partial x_j}{\partial z}L_{a_j} + L_f\right)^{\sigma-1} h(x)b^i(z)\right]^{-1}$$

$$\left\{v^i - \mathcal{C}^i h(x) - \sum_{\nu=1}^{\sigma}\mathcal{C}^i\gamma_\nu \left(\sum_{j=1}^{n}\frac{\partial x_j}{\partial z}L_{a_j} + L_f\right)^{\nu} h(x)\right\}$$

DISTRIBUTED STATE FEEDBACK CONTROL

1 Enforces the following input/output response in the closed-loop system:

$$\gamma_\sigma \frac{d^\sigma \bar{y}^i}{dt^\sigma} + \cdots + \gamma_1 \frac{d\bar{y}^i}{dt} + \bar{y}^i = v^i$$

2 Guarantees local closed-loop stability if:

◇ The roots of the equation

$$1 + \gamma_1 s + \cdots + \gamma_\sigma s^\sigma = 0$$

lie in the open left-half of the complex plane.

◇ The zero dynamics is locally exponentially stable.

DISTRIBUTED OUTPUT FEEDBACK CONTROL
Christofides and Daoutidis, AIChE J., 1996

- Combination of distributed state feedback and state observers

- State observer :

$$\frac{\partial \eta}{\partial t} = A\frac{\partial \eta}{\partial z} + f(\eta) + g(\eta)\sum_{i=1}^{l}\left(H(z-z_i) - H(z-z_{i+1})\right) b^i(z)\bar{u}^i(t)$$

$$+\sum_{i=1}^{l}\left(H(z-z_i) - H(z-z_{i+1})\right) \mathcal{P}^i(\bar{y}^i - \mathcal{C}^i k(z)\eta)$$

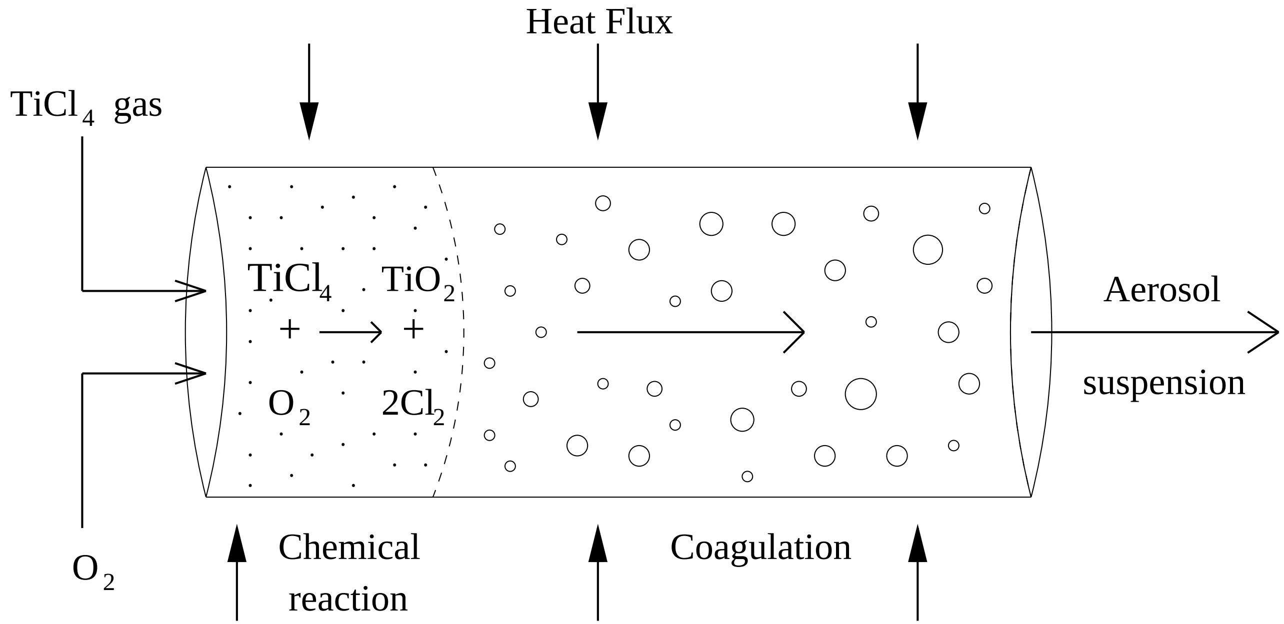
- The eigenvalues of the operator $\bar{\mathcal{L}}^i = A\dfrac{\partial}{\partial z} + B(z) - \mathcal{P}^i\mathcal{C}^i k(z)$ lie in the left-half plane

APPLICATION TO A TITANIA AEROSOL REACTOR

- Aerosol reactor used to produce TiO_2, according to:

$$TiCl_4(g) + O_2(g) \rightarrow TiO_2(s) + 2Cl_2(g)$$

- Schematic of the process:



- Chemical reaction and nucleation cannot be distinguished.
- Brownian and turbulent coagulation determine particle size.

PROCESS MODEL

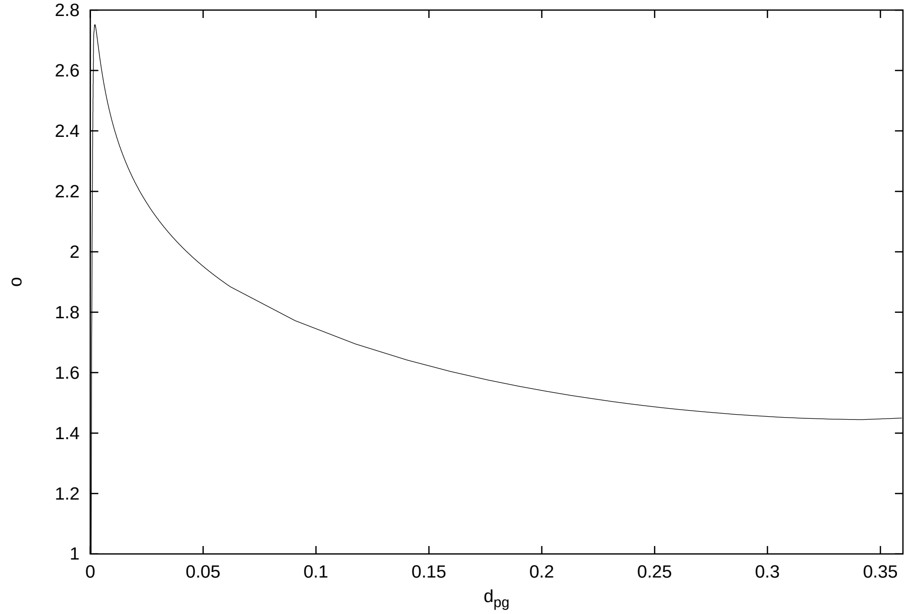
- Process model (lognormal size distribution):

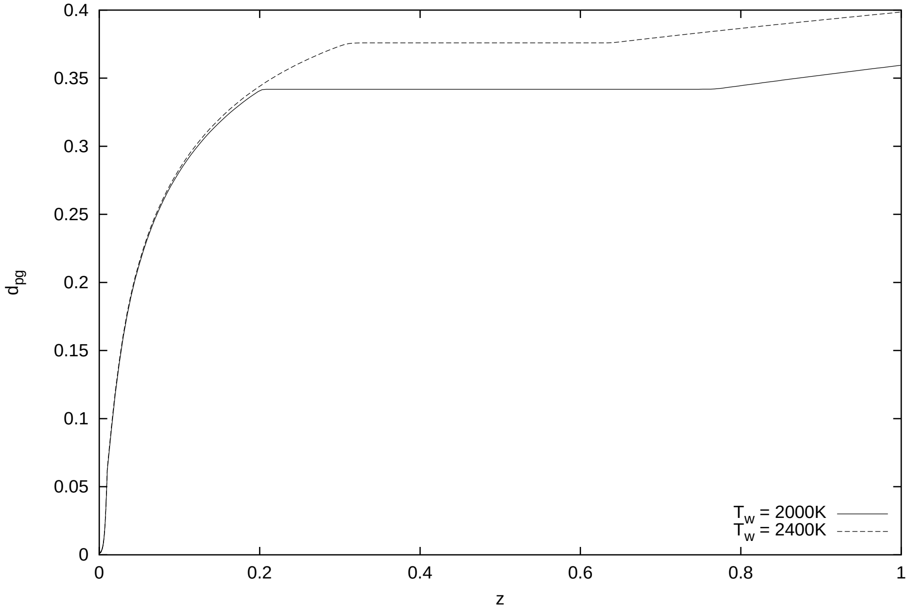
$$
\begin{aligned}
\frac{\partial N}{\partial \theta} &= -\phi \frac{\partial(\bar{v}_z N)}{\partial \bar{z}} + k' x_1 - \xi N^2 \\
\frac{\partial V}{\partial \theta} &= -\phi \frac{\partial(\bar{v}_z V)}{\partial \bar{z}} + k' x_1 \\
\frac{\partial V_2}{\partial \theta} &= -\phi \frac{\partial(\bar{v}_z V_2)}{\partial \bar{z}} + k' x_1 + 2\zeta V^2 \\
\frac{\partial \bar{C}_i}{\partial \theta} &= -\phi \frac{\partial(\bar{v}_z \bar{C}_i)}{\partial \bar{z}} + \alpha_i k' \bar{C}_i, \quad i = 1, .., 3 \\
\frac{\partial \bar{T}}{\partial \theta} &= -\phi \frac{\partial(\bar{v}_z \bar{T})}{\partial \bar{z}} + \left[A k' \bar{C}_1 + B(\bar{T}_w - \bar{T}) \right] \bar{C}_{pv}^{-1} \\
\frac{\partial \bar{v}_z}{\partial \theta} &= -\phi \bar{v}_z \frac{\partial \bar{v}_z}{\partial \bar{z}} + E \bar{v}_z^2
\end{aligned}
$$

$\bar{C}_1, \bar{C}_2, \bar{C}_3$	:	dimensionless concentrations of $TiCl_4$, O_2 and Cl_2
$\bar{T}, \bar{T}_w$	:	dimensionless process and wall temperatures
A_1, A_2, B, C, E	:	dimensionless constants

SPECIFICATION OF THE CONTROL PROBLEM

- Optimal reactor design to minimize product polydispersity (left figure).
- Effect of wall temperature on geometric average particle diameter (right figure).
- Controlled output: v_g at the outlet of the reactor;
  Manipulated input: T_w.

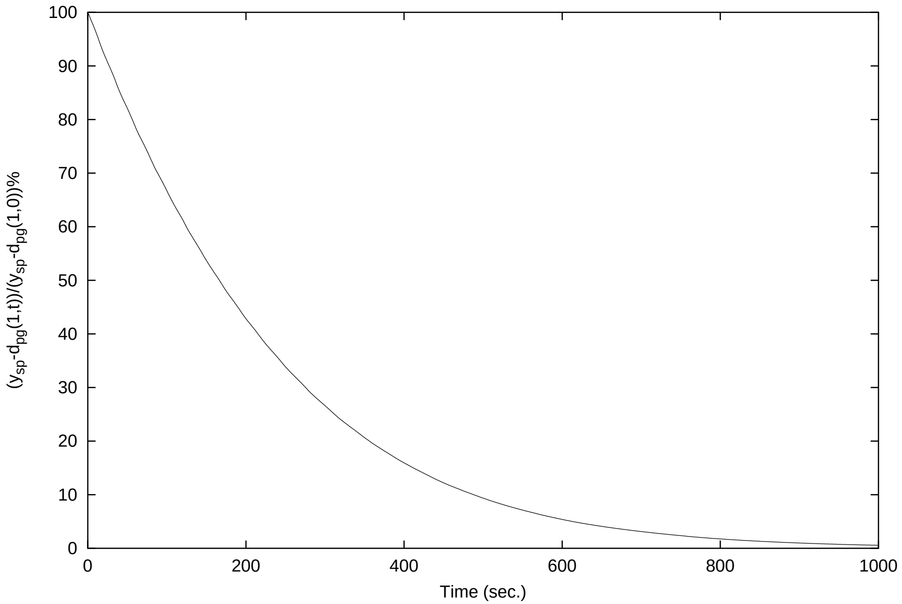


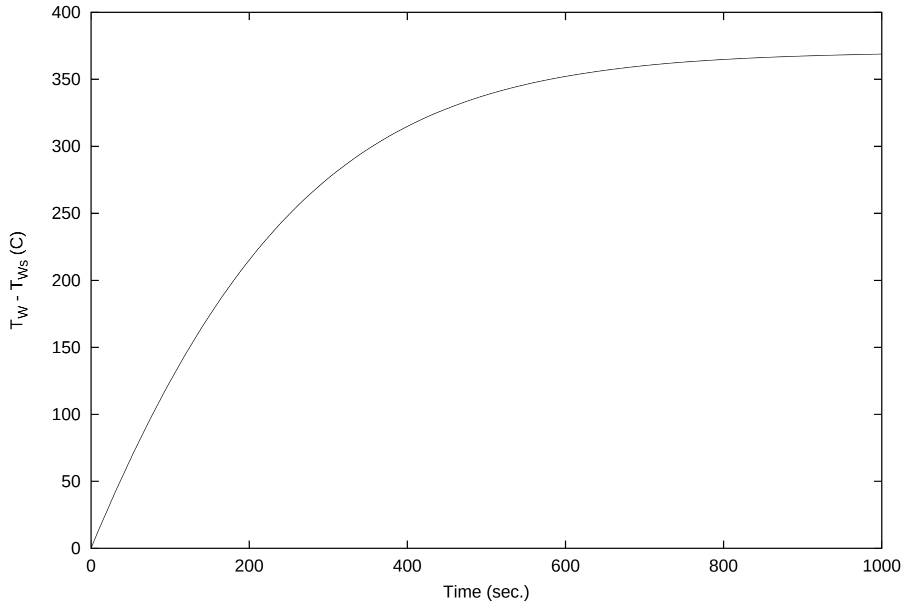


CLOSED-LOOP SIMULATION RESULTS

Nominal case

- Closed-loop profile of v_g in the outlet of the reactor under nonlinear control(left figure).
- Manipulated input profile under nonlinear control (right figure).

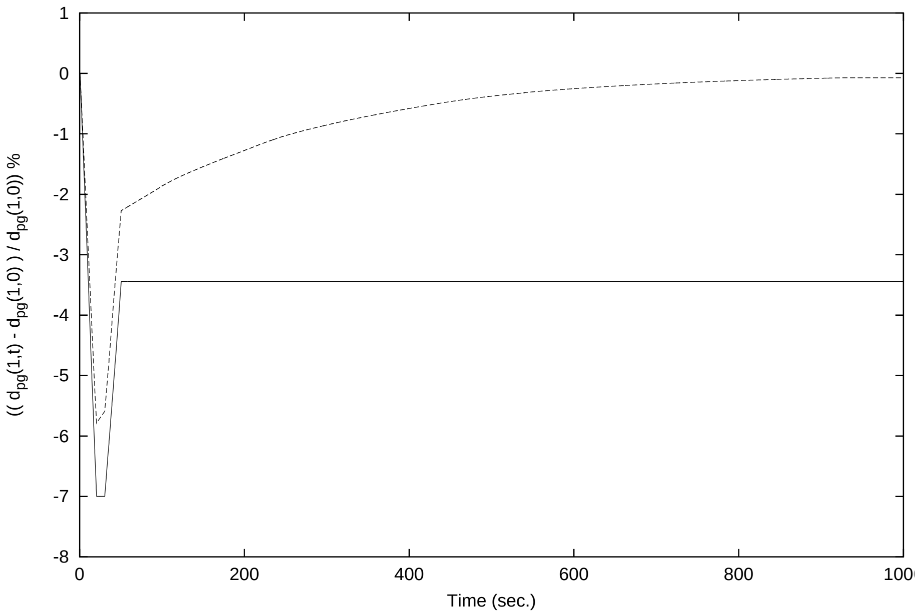


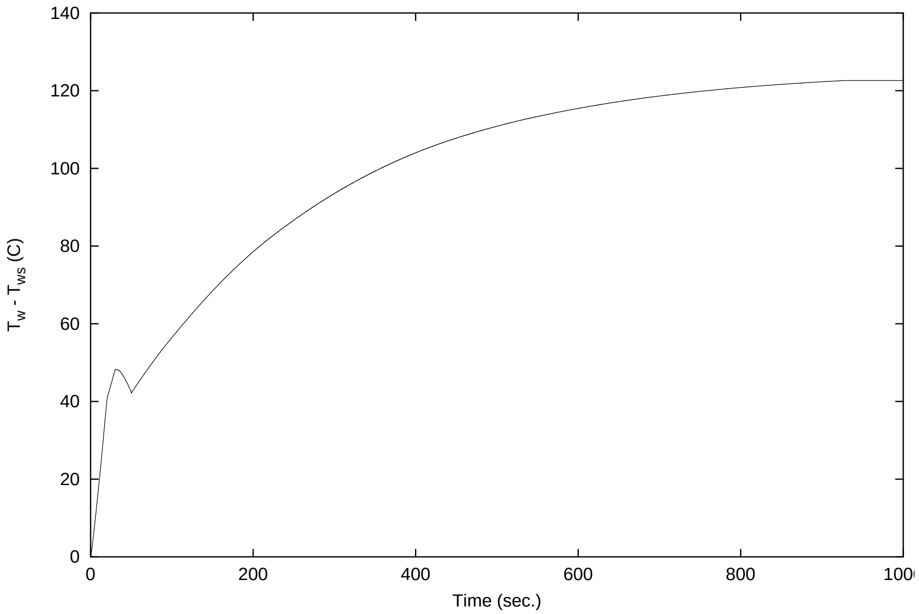


CLOSED-LOOP SIMULATION RESULTS

Unmeasured disturbances in parallel

- Open-loop profile and closed-loop profile of v_g in the outlet of the reactor under nonlinear control (left figure).
- Manipulated input profile under nonlinear control (right figure).

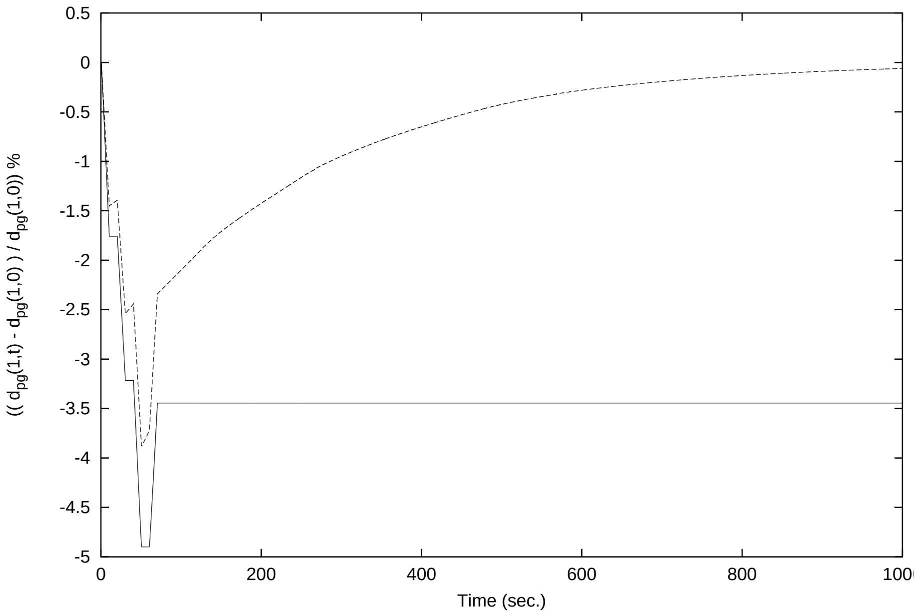


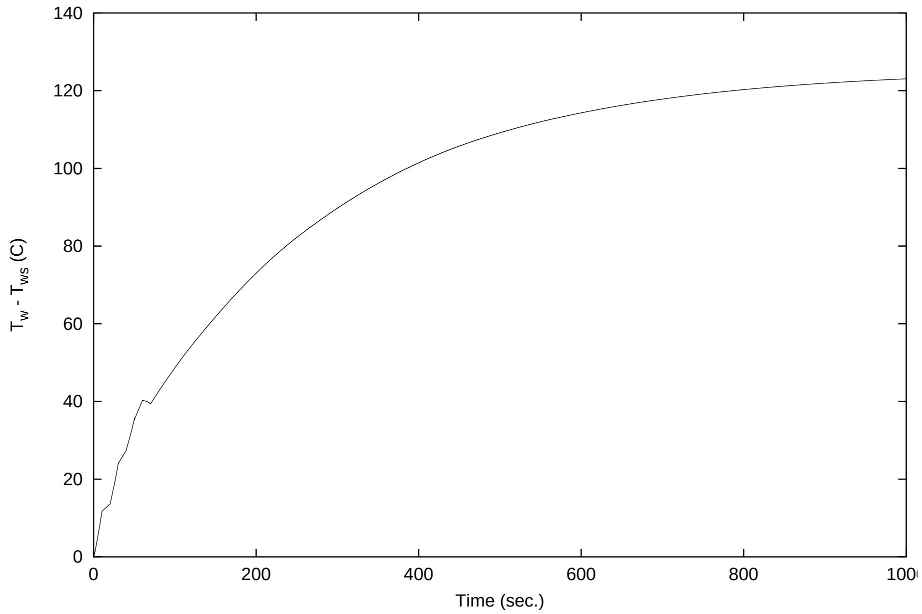


CLOSED-LOOP SIMULATION RESULTS

Unmeasured disturbances in series

- Open-loop profile and closed-loop profile of v_g in the outlet of the reactor under nonlinear control (left figure).
- Manipulated input profile under nonlinear control (right figure).

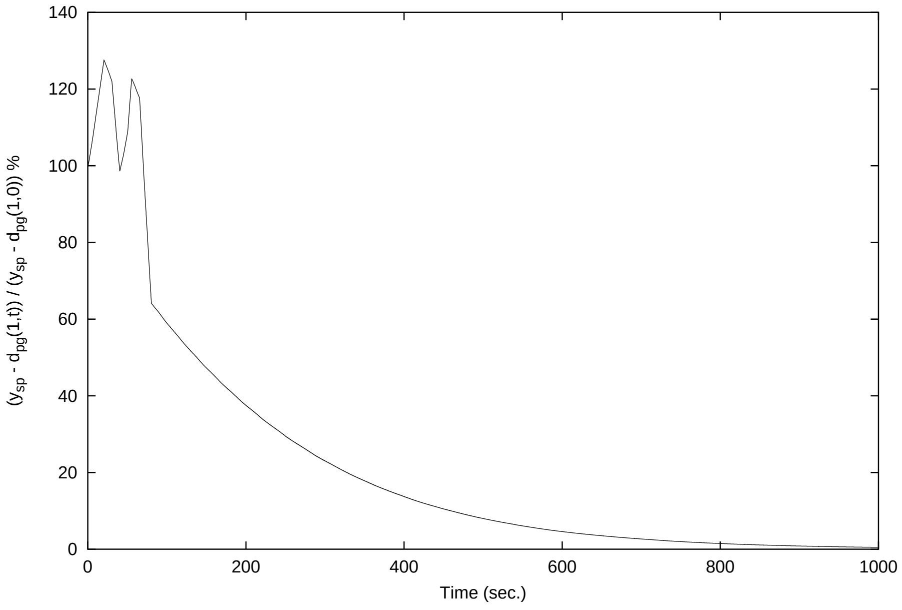


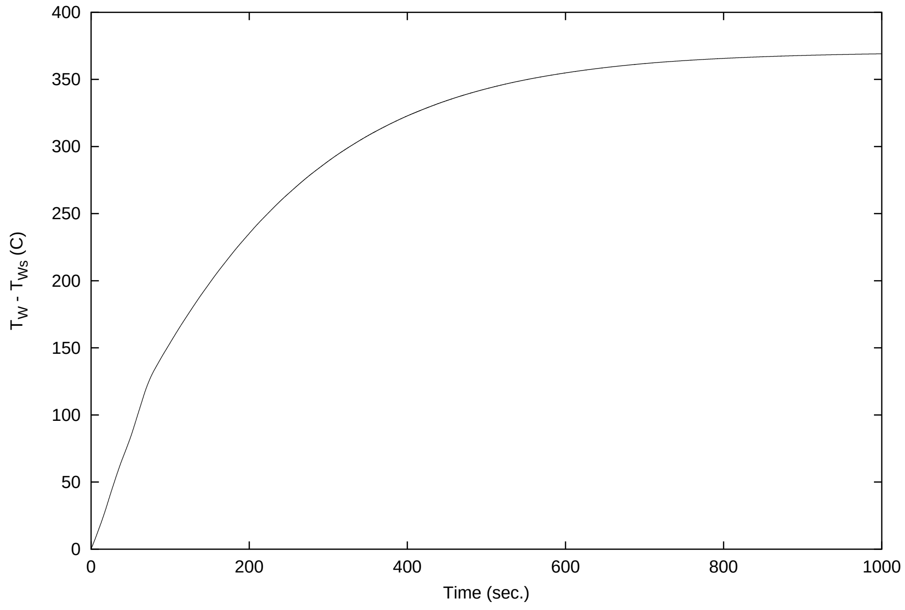


CLOSED-LOOP SIMULATION RESULTS

Unmeasured disturbances

- Closed-loop profile of v_g in the outlet of the reactor under nonlinear control(left figure).
- Manipulated input profile under nonlinear control (right figure).

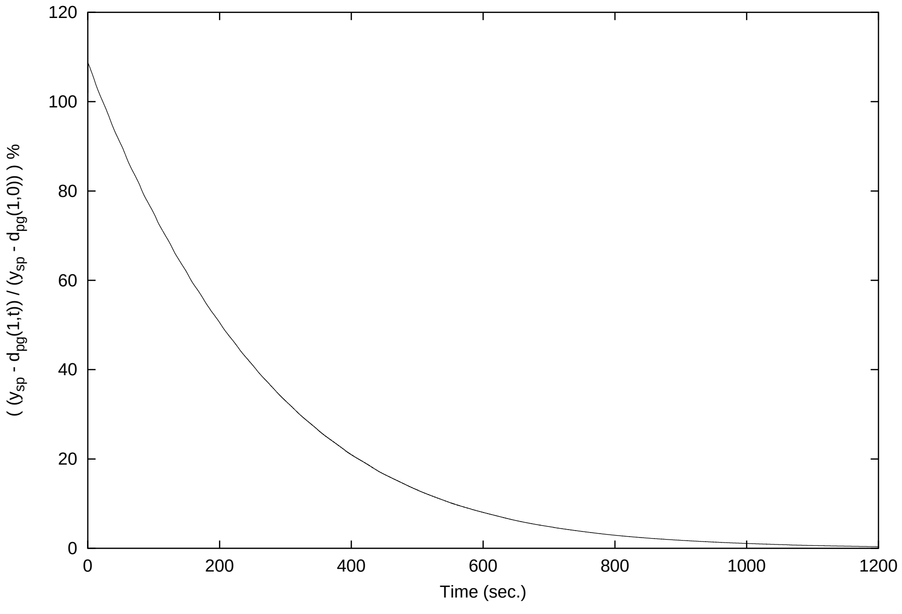


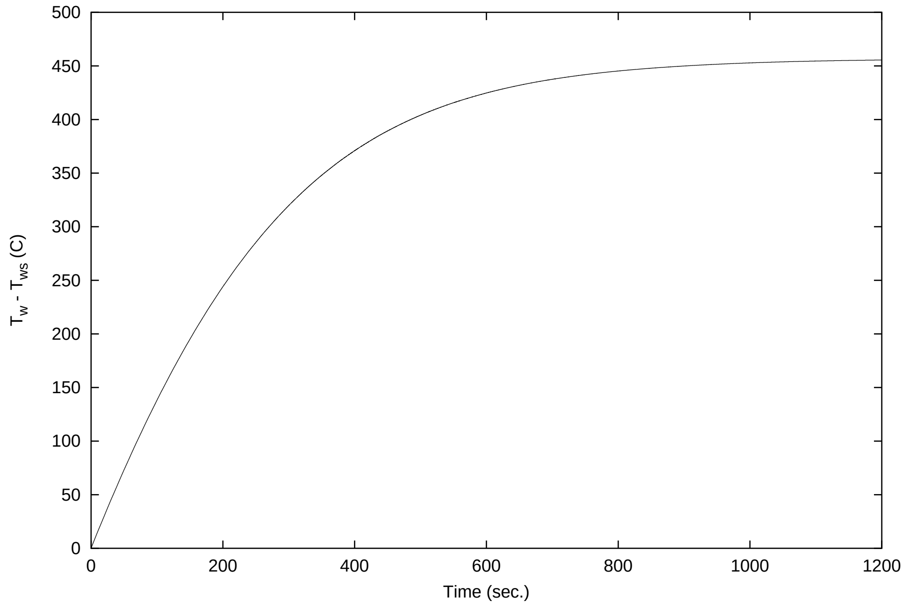


CLOSED-LOOP SIMULATION RESULTS

Parametric Uncertainty

- Closed-loop profile of v_g in the outlet of the reactor under nonlinear control (left figure).
- Manipulated input profile under nonlinear control (right figure).

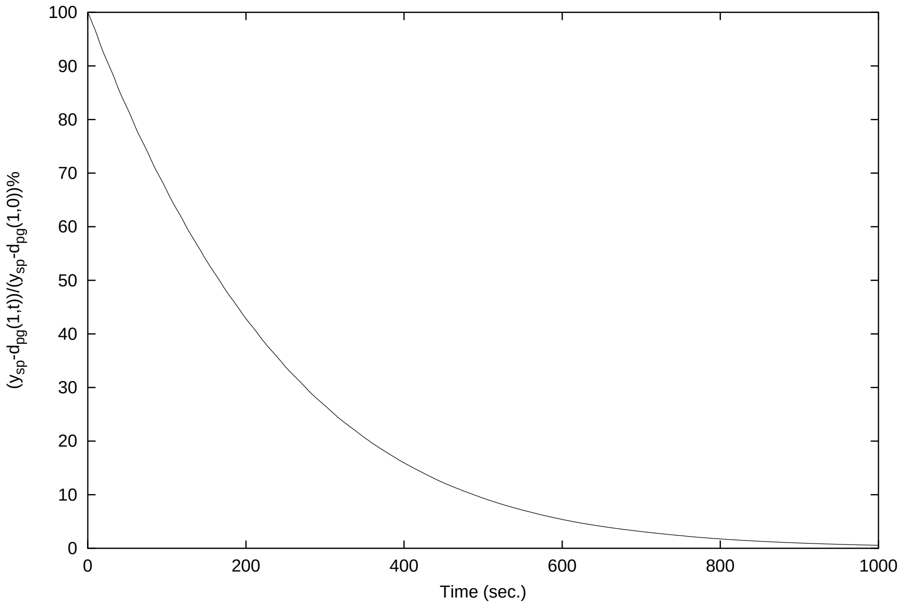


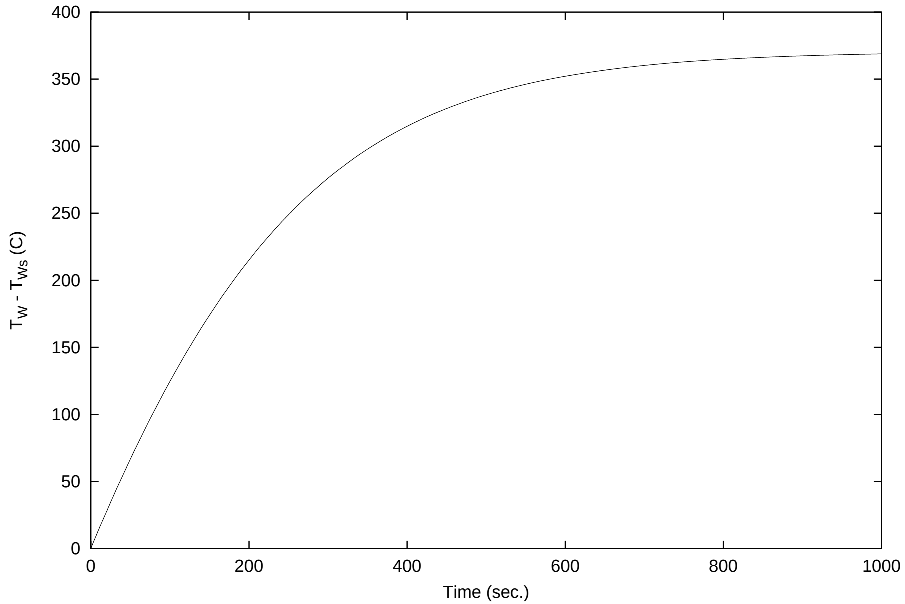


CLOSED-LOOP SIMULATION RESULTS

Unmodeled actuator dynamics

- Closed-loop profile of v_g in the outlet of the reactor under nonlinear control (left figure).
- Manipulated input profile under nonlinear control (right figure).





SUMMARY

- Methods for nonlinear order reduction and control for various classes of particulate process.
  - ◇ Model reduction
  - ◇ Model-based controller design
    - ▷ Geometric, Lyapunov-based and Model Predictive Control
    - ▷ Control relevant problems:
      - ⋆ Nonlinearity
      - ⋆ Uncertainty
      - ⋆ Constraints
      - ⋆ State measurements
- Applications to complex particulate processes.
  - ◇ Control of size distribution in crystallization.
  - ◇ Seeded batch crystallizer.
  - ◇ Aerosol Titania reactor.

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