

**This document must be cited according to its final version
which was presented in a conference as:**

**P. Dufour, D. Edouard, H. Hammouri,
"Multivariable control of a catalytic reverse flow reactor:
Comparison between LQR and MPC approaches",
ChemCon'04-First joint meeting of American Institute of Chemical
Engineers (AIChE) and Indian Institute of Chemical Engineers (IICChE),
Mumbai, India, december 27-30, 2004.**

**All open archive documents of Pascal Dufour are available:
<http://hal.archives-ouvertes.fr/DUFOUR-PASCAL-C-3926-2008>**

**The list of Pascal Dufour's works published in journals are available:
<http://www.researcherid.com/rid/C-3926-2008>**

**Multivariable Control of a
Catalytic Reverse Flow Reactor:
Comparison between LQR and MPC Approaches**

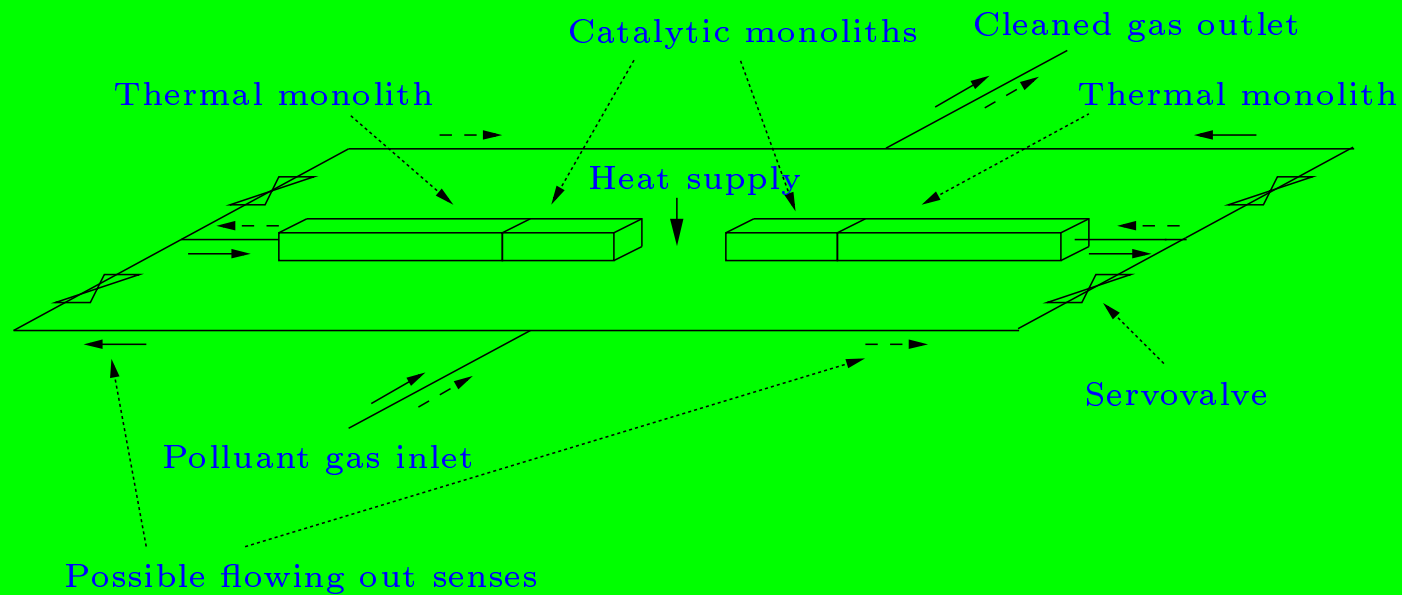
Co-authors: **Dufour P.** (speaker), Edouard D. & Hammouri H.

LAGEP University Claude Bernard Lyon 1-UMR CNRS 5007, France

Outline

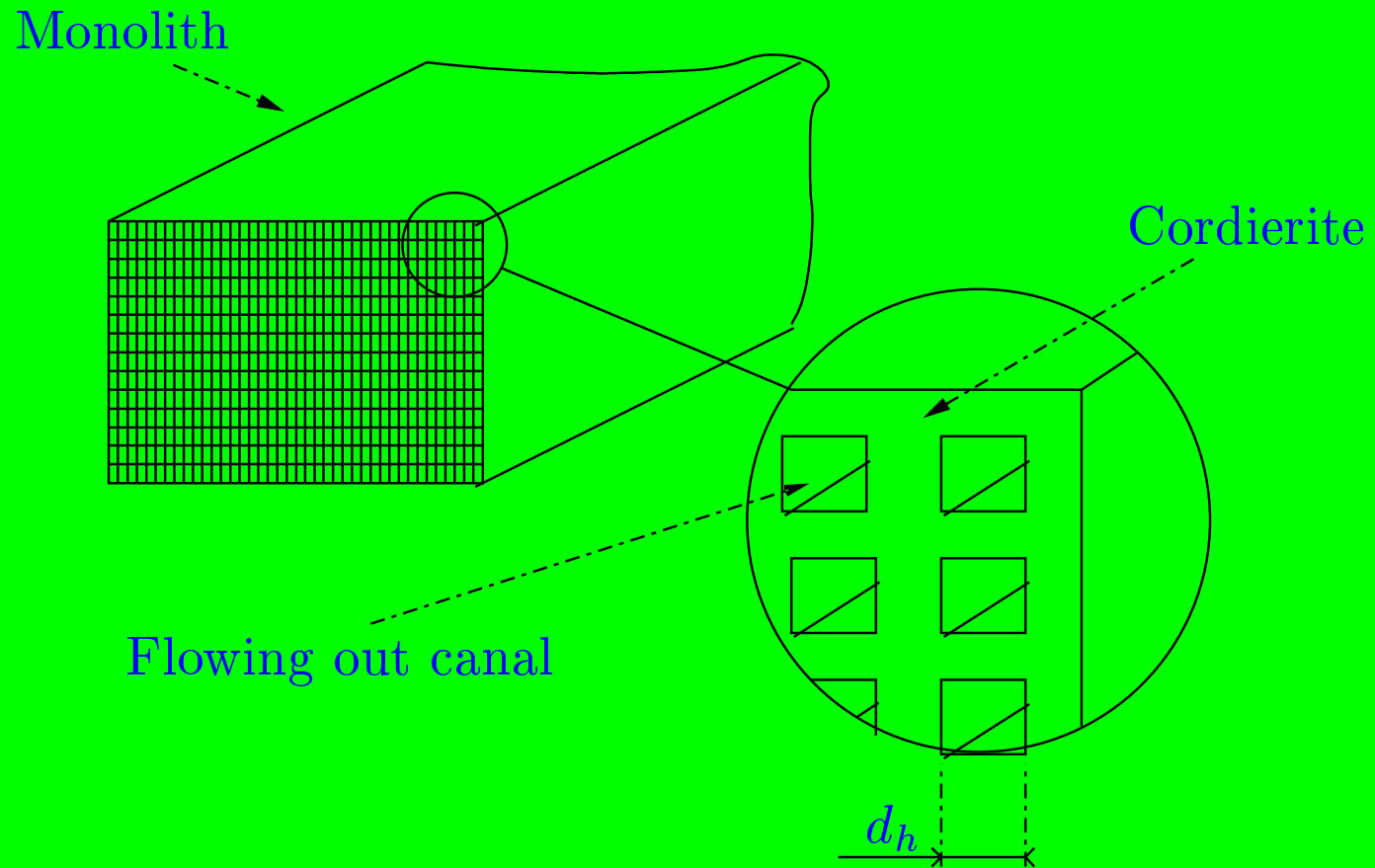
- Catalytic reverse flow reactor (RFR): description and control issues
- Model description
- Observer synthesis
- Control objective: Compare LQR and MPC performances
 - Provide real-time multivariable controllers for a RFR such that:
 - * concentration of pollutant released at the inlet stay below a threshold,
 - * limiting operating conditions are accounted for,
 - * optimize the use of the control actions.
 - LQR design and simulation results
 - MPC design and simulation results
- Conclusions

Principle scheme for the catalytic RFR



Monolith section

Cordierite monoliths of square cross sections (1*1 mm) channels:



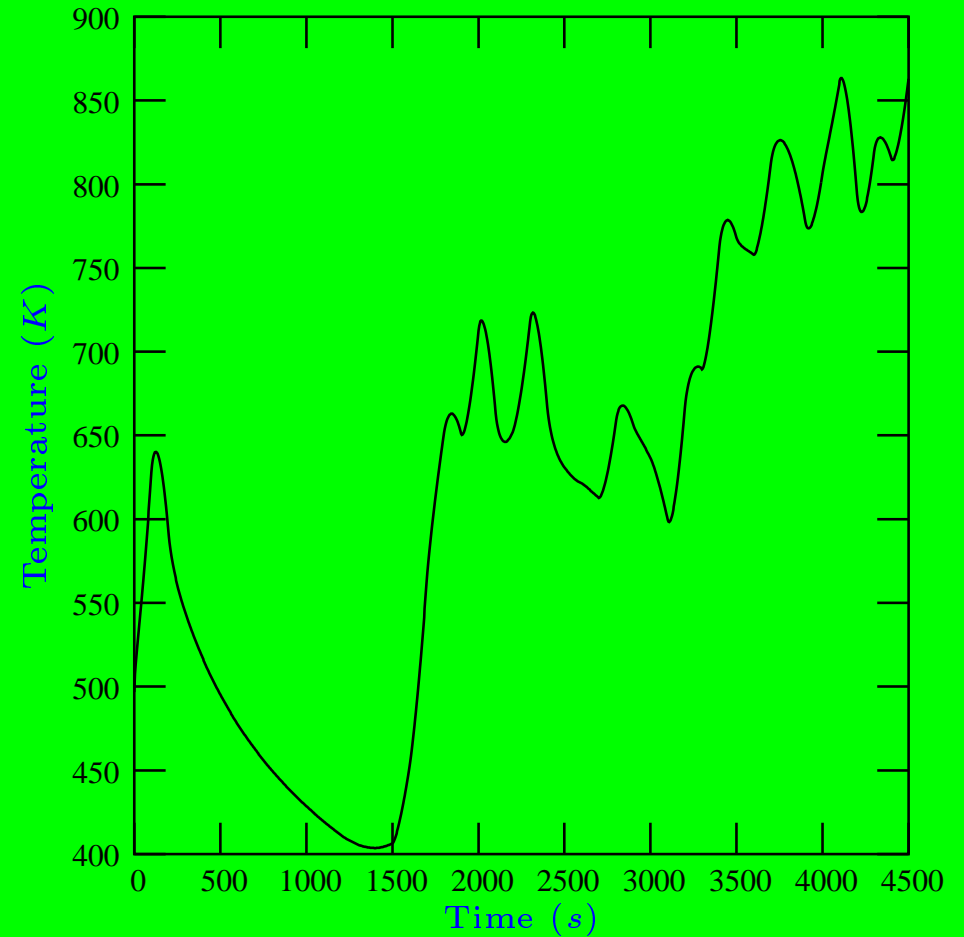
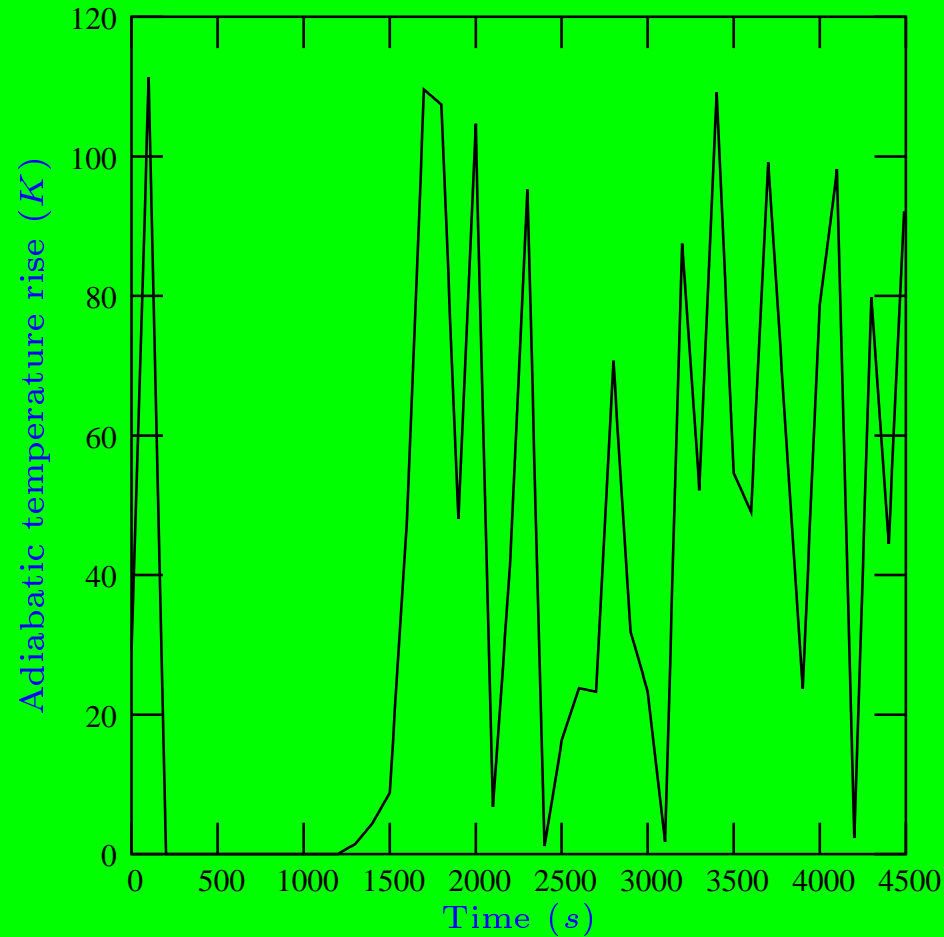
- **Monolith** in the core region is **catalytically active** and is **inert** in both end sections.
- Through **periodic flow reversal**, **heat released by reaction** is first trapped in the packing and then used to **heat up the feed**. Therefore, high temperatures exist in catalyst bed whereas the inlet and outlet gas stream (VOC) have ambient temperature.
- In the core region, an **electric heater** maintains ignition temperature, while the temperature in the catalytic layer is decreased by **fresh air dilution**.
- A blower located downstream of the RFR keeps aspiration of the pollutant at a **constant flow rate**.
- The packed layer is **adiabatic**, **except** in the core region where **heat loss** is inevitable due to both the installation for air dilution and the high temperature in this region.
- **Highest temperature** is located at the **inlet of catalytic monoliths**.

Various behaviours of the RFR: control issues

According to the **operating conditions**, various behaviours are possible:

- If **feed of pollutant concentration is too rich**: release of heat due to the reaction produces **thermal overheating** that deteriorates the catalysts. Temperature inside the reactor has therefore to be **maintained under $600K$** [Ramdani et al., 2001].
- If **feed of pollutant concentration is too lean**: low heat released during the reaction leads to the **extinction of the reactor**. Temperature inside the reactor has therefore to be **maintained over $450K$** [Ramdani et al., 2001].
- If the **feed of pollutant concentration** is such that the reaction temperature falls **within an envelope** outlined by the two previous boundary temperatures: **autothermal operation** is reached and **no control action** would be required.

Hot spot temperature without control



Input disturbance (left) and uncontrolled hot spot temperature (right).

Overview of RFR control (1)

- Various ideas have been proposed to provide efficient means of **temperature control**:
 - [Niesen et al., 1995] to **suppress temperature run-away** when rich feed: **cold gas injection**, hot gas withdrawing or heat recovery through internal heat exchangers;
 - [Cunill et al., 1997] to **prevent extinction** for lean feed: hot gas supply or **internal heating**.
- [Budman et al., 1996] was the **first complete study on RFR control**: a parametric study allows characterizing the use of 2 RFR MVs: coolant flow rate and cycle time. 2 SISO controllers (MV=coolant flow rate) assume that the **temperature and the concentration at the RFR inlet** were **constant input disturbances**: use of PID and a feed forward controller which is not usable during transient conditions.

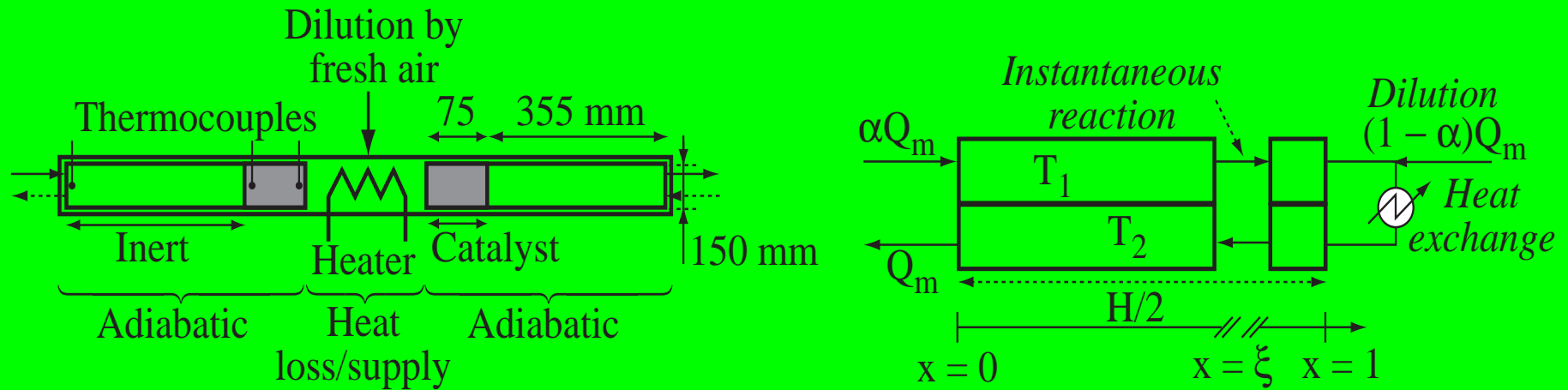
Overview of RFR control (2)

- [Keith, 2003]: to avoid extinction and overheating, a simple switching control law strategy **tunes the switching time**.
- [Dufour et al., 2003]: **SISO MPC** optimizes the consumption of electrical power accounting for the **maximum amount of concentration pollutant released** at the outlet. Limitation was concerned with the **impossibilities to control overheating** and to handle **stochastic variations** of the inlet concentration.
- [Dufour et al., 2004]: **MIMO MPC** optimizes the consumption of electrical power and the dilution rate while **maintaining the hot spot temperature inside the prescribed enveloppe**. Limitation was concerned with the difficulties to handle **stochastic variations** of the inlet concentration. **Real time** control aspect becomes **critical**.

Modeling [Edouard & Hammouri, 2004]

- **Motivation:** the model is used in the optimal model based control framework and the observer synthesis. The current periodic model used [Ramdani et al., 2001] need a set of 800 DAE, and the sampling time is 10s: **accuracy and time spent for model calculation are critical.**
- The **new model** considered for control purpose is obtained from a **countercurrent pseudo-homogeneous model** [Edouard, Hammouri, 2004]):
 - Assume that the **kinetic reaction can be neglected** under strong mass transfer limitation,
 - Accounts for **periodic frequency correction**,
 - **1 nonlinear parabolic PDE**, 2 algebraic equations, and nonlinear boundary conditions,
 - Model **more accurate and faster** to solve than [Dufour et al., 2004]).

Modeling [Edouard & Hammouri, 2004]



Left: main geometrical characteristics of the RFR.

Right: the countercurrent model.

Notation: some elements [Edouard & Hammouri, 2004]

x = Normalized space variable [-]

T_s = Solid temperature [K]

T_{g1}, T_{g2} = Upstream and downstream gas temperature in the monolith [K]

T_0 = ambient temperature and feed temperature [K]

ω = VOC mass fraction [-]

θ = Period of flow reversal [s]

α = fraction of feed flow rate [-]:

- if $\alpha = 1$: no dilution
- if $\alpha = 0$: maximum dilution

Q_j = External power supply [W]

$\varphi(x)$ = Characteristic function of the catalytic monolith [-]:

- $\varphi(x) = 0$ in the inert monoliths ($x < \xi_\theta$)
- $\varphi(x) = 1$ in the catalytic monoliths ($x \geq \xi_\theta$)

N' = Number of transfer units for heat loss [-]

Modeling [Edouard & Hammouri, 2004]

Normalizing some variables, we obtain the nonlinear PDE model:

$$\begin{cases} \tau \frac{\partial T_s(x, t)}{\partial t} = \left(\frac{1}{P_{ax\theta}} + \frac{1 + \alpha^2}{2P_\theta} \right) \frac{\partial^2 T_s(x, t)}{\partial x^2} + \frac{1 - \alpha}{2} \frac{\partial T_s(x, t)}{\partial x} + P_\theta \Delta T_{ad}(t) \psi(x, t) \\ \alpha \frac{\partial \omega_1(x, t)}{\partial x} + P_\theta \omega_1(x, t) = 0, \quad - \frac{\partial \omega_2(x, t)}{\partial x} + P_\theta \omega_2(x, t) = 0 \end{cases} \quad (1)$$

with:

$$\begin{cases} P_\theta = \frac{ha_c H}{2\rho_0 u_{v0} c_{pmg}} \left(1 - \frac{\theta}{2\tau} \right), \quad \frac{1}{P_{ax\theta}} = \frac{2\lambda_{ax}^s}{(H\rho_0 u_{v0} c_{pmg}) \left(1 - \frac{\theta}{2\tau} \right)}, \\ \tau = \frac{(1 - \varepsilon)\rho_s c_{ps} H}{2\rho_0 u_{v0} c_{pmg}}, \quad x = \frac{z}{H/2} \\ \Delta T_{ad}(t) = \frac{\Delta H}{M c_{pmg}} \omega_{10}(t), \quad \psi(x, t) = \varphi(x) \frac{\omega_1(x, t) + \omega_2(x, t)}{2\omega_{10}(t)} \end{cases}$$

Modeling [Edouard & Hammouri, 2004]

The boundary condition at $x = 0$ is:

$$\begin{cases} \omega_1(x, t) = \omega_{10}(t) \\ T_{g1}(x, t) = T_s(x, t) - \frac{\alpha}{P_\theta} \frac{\partial T_s(x, t)}{\partial x} = T_0 \end{cases}$$

The boundary condition at $x = 1$ is:

$$\begin{cases} (1 + N')(T_{g2}(x, t) - T_0) = \alpha(T_{g1}(x, t) - T_0) + \frac{Q_j}{S\rho_0 u_{v0} C_{pmg}} \\ T_{g1}(x, t) = T_s(x, t) - \frac{\alpha}{P_\theta} \frac{\partial T_s(x, t)}{\partial x} \\ T_{g2}(x, t) = T_s(x, t) + \frac{1}{P_\theta} \frac{\partial T_s(x, t)}{\partial x} \\ \alpha\omega_1(x, t) = \omega_2(x, t) \end{cases}$$

Modeling [Edouard & Hammouri, 2004]

Initial conditions are at $t = 0$:

$$T_{g1}(x, t) = T_{g2}(x, t) = T_s(x, t) = T_0$$

The first term in the right hand side of (1) involves an effective axial heat conductivity given by:

$$\left\{ \begin{array}{l} \frac{1}{P_{ax\theta}} + \frac{1 + \alpha^2}{2P_\theta} = \frac{\lambda_{eff}}{\rho_0 u_{v0} c_{pmg} H / 2 \left(1 - \frac{\theta}{2\tau}\right)} \\ \lambda_{eff} = \lambda_{ax}^s + \frac{1 + \alpha^2}{2} \frac{(\rho_0 u_{v0} c_{pmg})^2}{ha_c} \end{array} \right. \quad (2)$$

When there is no dilution ($\alpha = 1$), λ_{eff} reduces to the well-known estimate of [Vortmeyer & Schaefer, 1974] as used by Niesen [Niesen et al., 1995].

This model experimentally matches the process behaviour during open-loop control and identification [Edouard & Hammouri, 2004].

Observer [Edouard & Hammouri, 2004]

An observer has to be designed since:

- The **input disturbance** (inlet VOC concentration) has a more realistic stochastic behaviour than in the previous RFR control studies, and **has a large influence over the process behavior**,
- The LQR formulation **needs the temperature profile**,
- The MPC **needs the input disturbance**.

The **input disturbance** and the **temperature profile** in the RFR are **estimated on-line using a high gain observer based on three temperatures measurements** [Edouard & Hammouri, 2004].

LQR formulation

Since it seems **natural to avoid heating and cooling at the same time**, **2 cost functions** are considered (based on the linearized model):

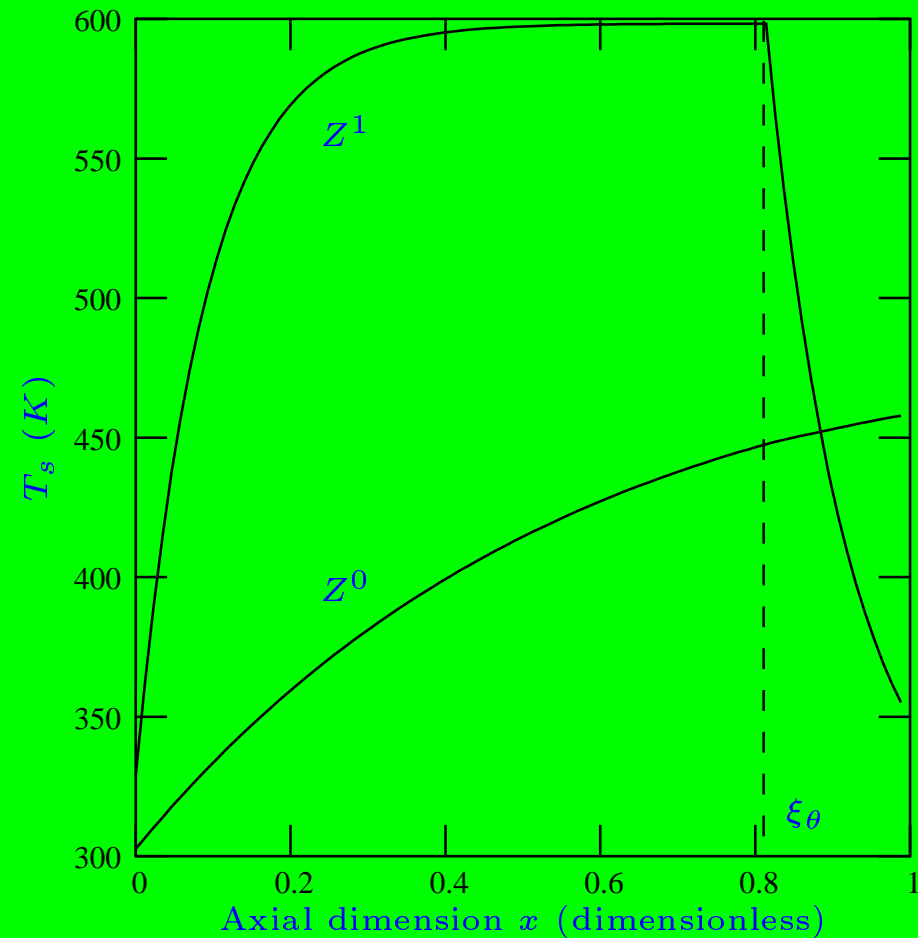
- When the **pollutant concentration is too low**, the **LQR** tunes ΔQ_j such that the temperature is kept over a $450K$:

$$\int_0^{\infty} (p_1^0(\Delta X(t))^2 + p_2^0(\Delta Q_j(t))^2) dt$$

- When the **pollutant concentration is too high**, the **LQR** tunes $\Delta \alpha$ such that the temperature is kept below $600K$:

$$\int_0^{\infty} (p_1^1(\Delta X(t))^2 + p_2^1(\Delta \alpha(t))^2) dt$$

LQR formulation: model linearizations

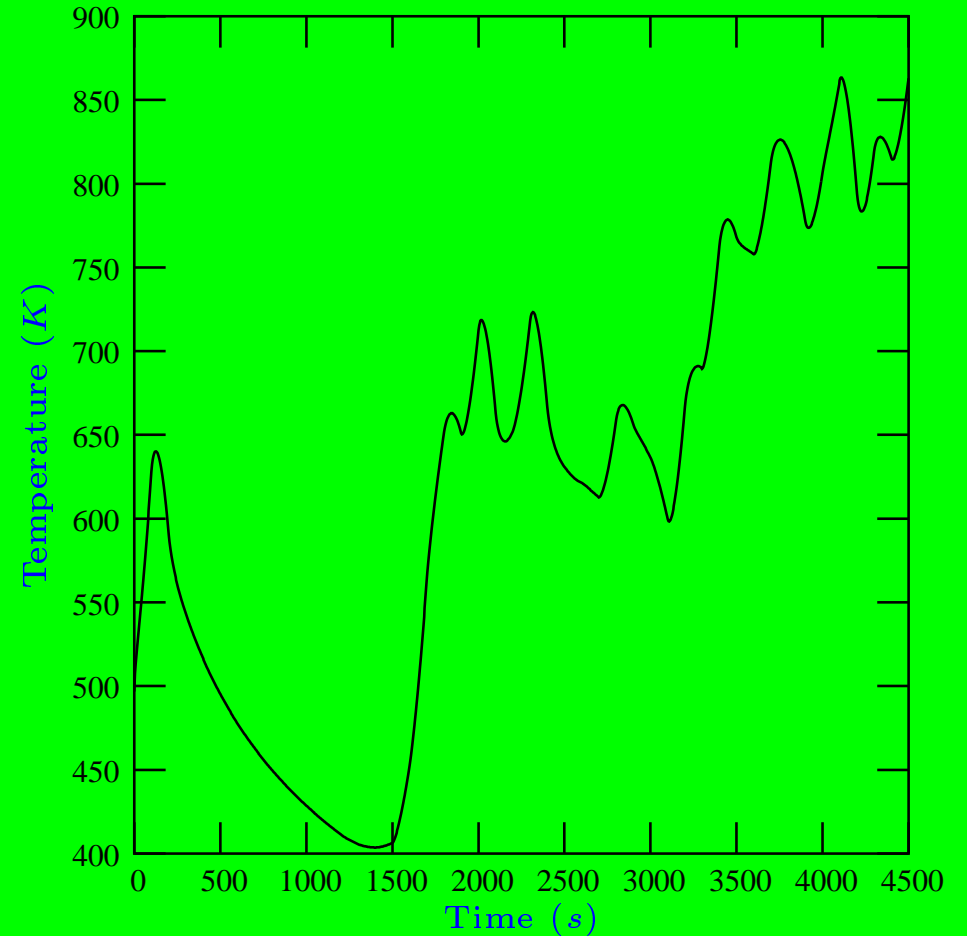
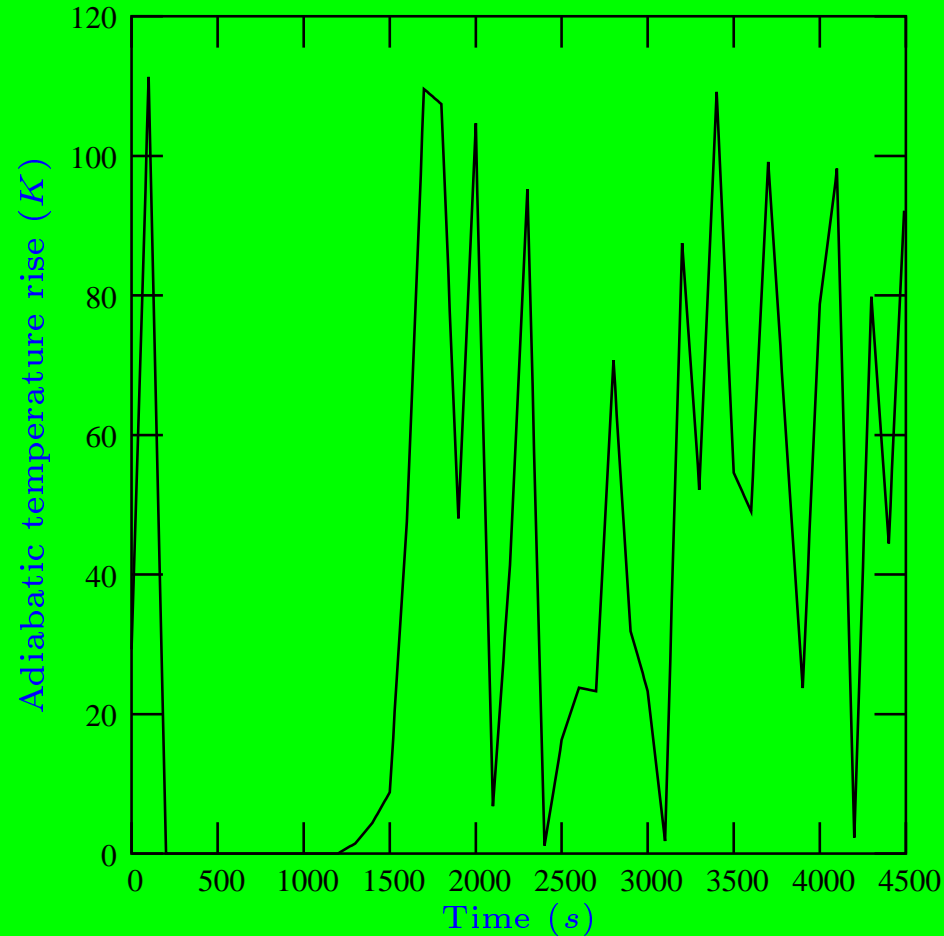


Linearized models are: $\Delta \dot{X}(t) = A(\alpha^i) \Delta X(t) + B_1^i \Delta \alpha(t) + B_2^i \Delta Q_j(t)$

LQR formulation

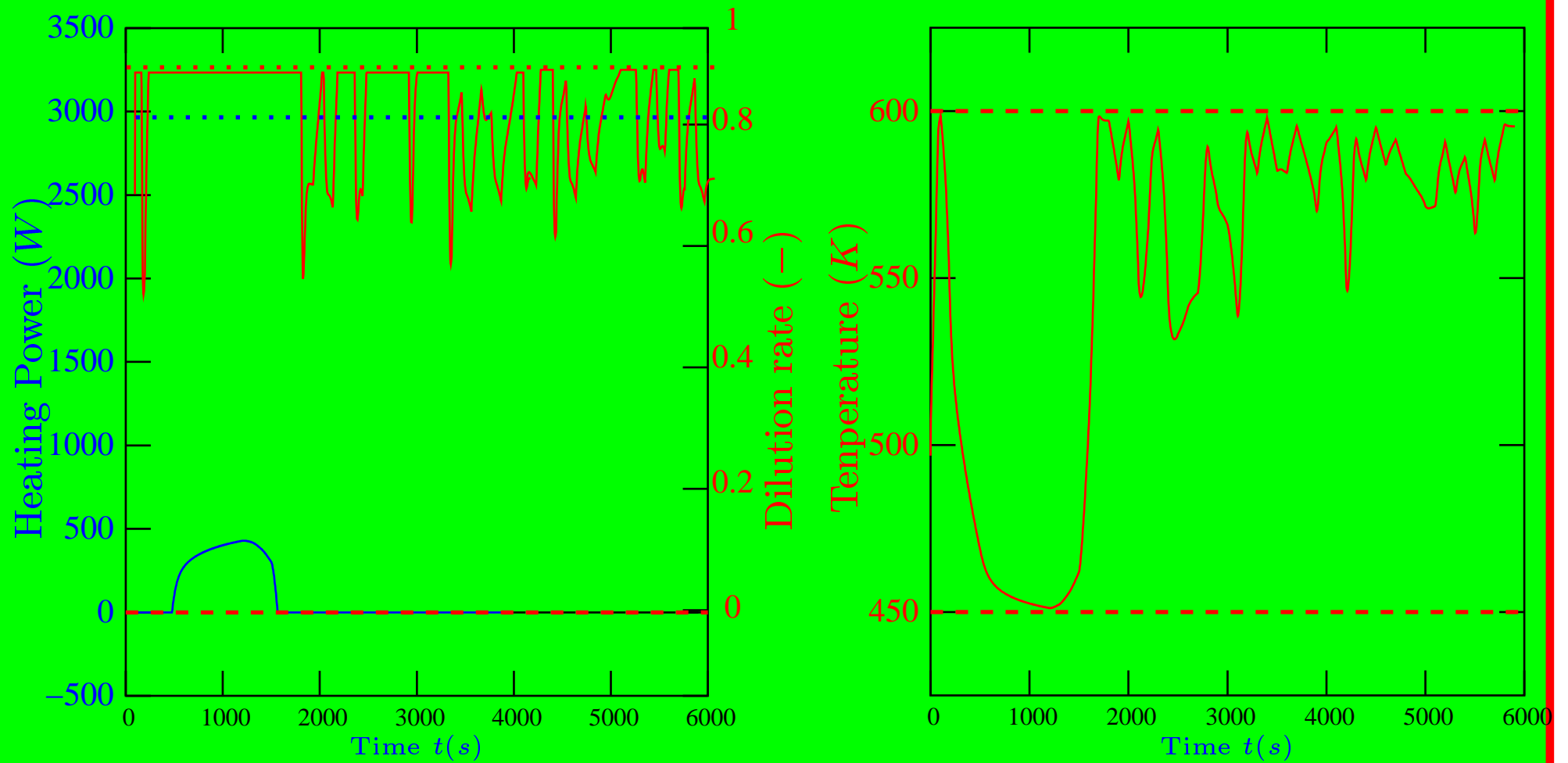
- In both cases, the control obtained from the minimization of these cost functions is a linear feedback of the form $\Delta Q_j(t) = -F^0 \Delta X$ or $\Delta \alpha(t) = -F^1 \Delta X$ with $\Delta X = X_e(t) - Z^i$ where ($i = 0, 1$), $X_e(t)$ is the estimate state given by the observer and each steady state is Z^i .
- The gains of the feedback matrix are obtained from the solution of the classical algebraic Riccati equation.

Hot spot temperature without control (reminder)



Input disturbance (left) and uncontrolled hot spot temperature (right).

LQR: simulation results



MPC formulation: model linearizations

To decrease the on-line computational burden, the model is linearized about the nominal nonlinear model with variations s.t.:

$$\begin{cases} Q_j(k) = Q_{j,0}(k) + \Delta Q_j(k) \\ \alpha(k) = \alpha_0(k) + \Delta\alpha(k) \\ X(k) = X_0(k) + \Delta X(k) \end{cases}$$

The linearized model used in the MPC is:

$$\Delta\dot{X}(t) = A(\alpha_0, Q_0, X_0)\Delta X(t) + B_1(\alpha_0, Q_0, X_0)\Delta\alpha(t) + B_2(\alpha_0, Q_0, X_0)\Delta Q_j(t)$$

MPC formulation [Dufour & Touré, 2004]

The MPC formulation is:

$$\min_{\Delta Q_j(k), \Delta \alpha(k)} J(\Delta Q_j(k), \Delta \alpha(k)) = (w_Q \left[\frac{Q_j(k) - Q_{j.\min}}{Q_{j.\max} - Q_{j.\min}} \right]^2 + w_\alpha \left[\frac{\alpha(k) - \alpha_{\max}}{\alpha_{\max} - \alpha_{\min}} \right]^2)$$

with constraints on MVs magnitude:

$$Q_{j.\min} = 0W \leq Q_j(j) = Q_{j.0}(j) + \Delta Q_j(j) \leq Q_{j.\max} = 3000W$$

$$\Delta \alpha_{\min} = 0 < \alpha(j) = \alpha_0(j) + \Delta \alpha(j) \leq \Delta \alpha_{\max} = 0.95$$

with 2 constraints c_i on the estimated state:

$$c_1(X(j), Q_j(j), \alpha(j)) = T_{s.\min} - T_s(x_{101}, j) \leq 0 \quad (j \in \{k + hp_1^i, k + hp_1^f\})$$

$$c_2(X, Q_j(j), \alpha(j)) = T_s(x_{101}, j) - T_{s.\max} \leq 0 \quad (j \in \{k + hp_2^i, k + hp_2^f\})$$

MPC formulation [Dufour & Touré, 2004]

- k =actual discrete time index, j =discrete time index.
- w_Q and w_α are positive weights.
- In order to decrease the computational burden, the **tuning of the control horizon is one**. Even if it is true that this tuning reduces strongly the degrees of freedom to solve the optimization problem, it **allows decreasing the computational time**, which is an important issue here.
- **Tuning parameters are the horizons:** hp_1^i and hp_1^f (resp. hp_2^i and hp_2^f) are the initial and future prediction horizons describing the lower (resp. upper) temperature constraint.

MPC: Tuning of the horizons

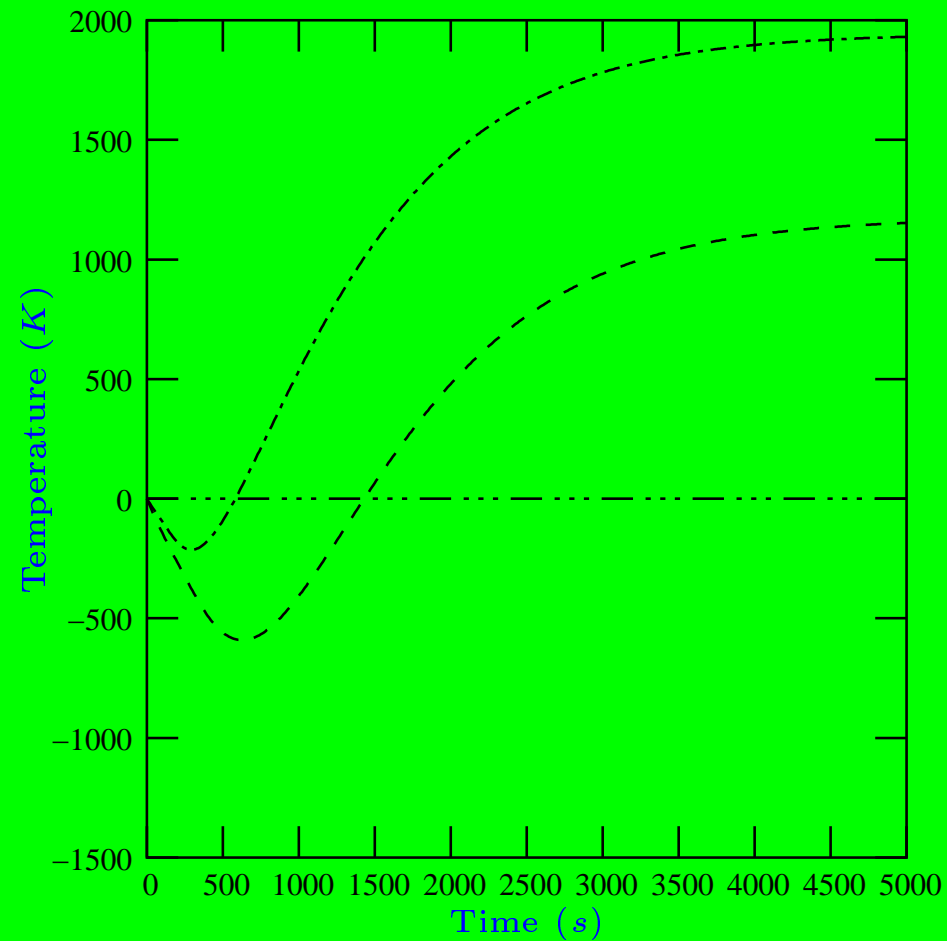
It is clear that the tuning of the controller parameters directly influences the constrained optimization problem and therefore closed-loop control results, since:

- This constrained optimization problem uses the **estimation of the input disturbance** (the adiabatic temperature rise ΔT_{ad}) which has an **evident impact over the closed-loop performances** (especially the constraints satisfaction).
- The **non-minimum phase behavior** of the process has to be handled.

Regarding the **impact of the input disturbance** over the optimization task and the constraints satisfaction required, some **guidelines for the tuning** of the controller parameters are first given.

Non-minimum phase behavior

Time evolution of 2 distributed sensitivities of T_s w.r.t. α :



MPC: Tuning of the initial horizon prediction

- The cooling action creates a non-minimum phase behaviour in the temperature involved in output constraints. Therefore, initial prediction horizon has to be tuned sufficiently large such that this behaviour is not accounted for into the controller, especially when constraints are saturated.

Conclusion: a sufficiently large initial prediction horizon is required.

- If some constraints are currently saturated, they may **no more be satisfied** in the **very close future** due to possible strong variations of ΔT_{ad} .

Conclusion: the smallest initial prediction horizon is required.

MPC: Tuning of the final horizon prediction

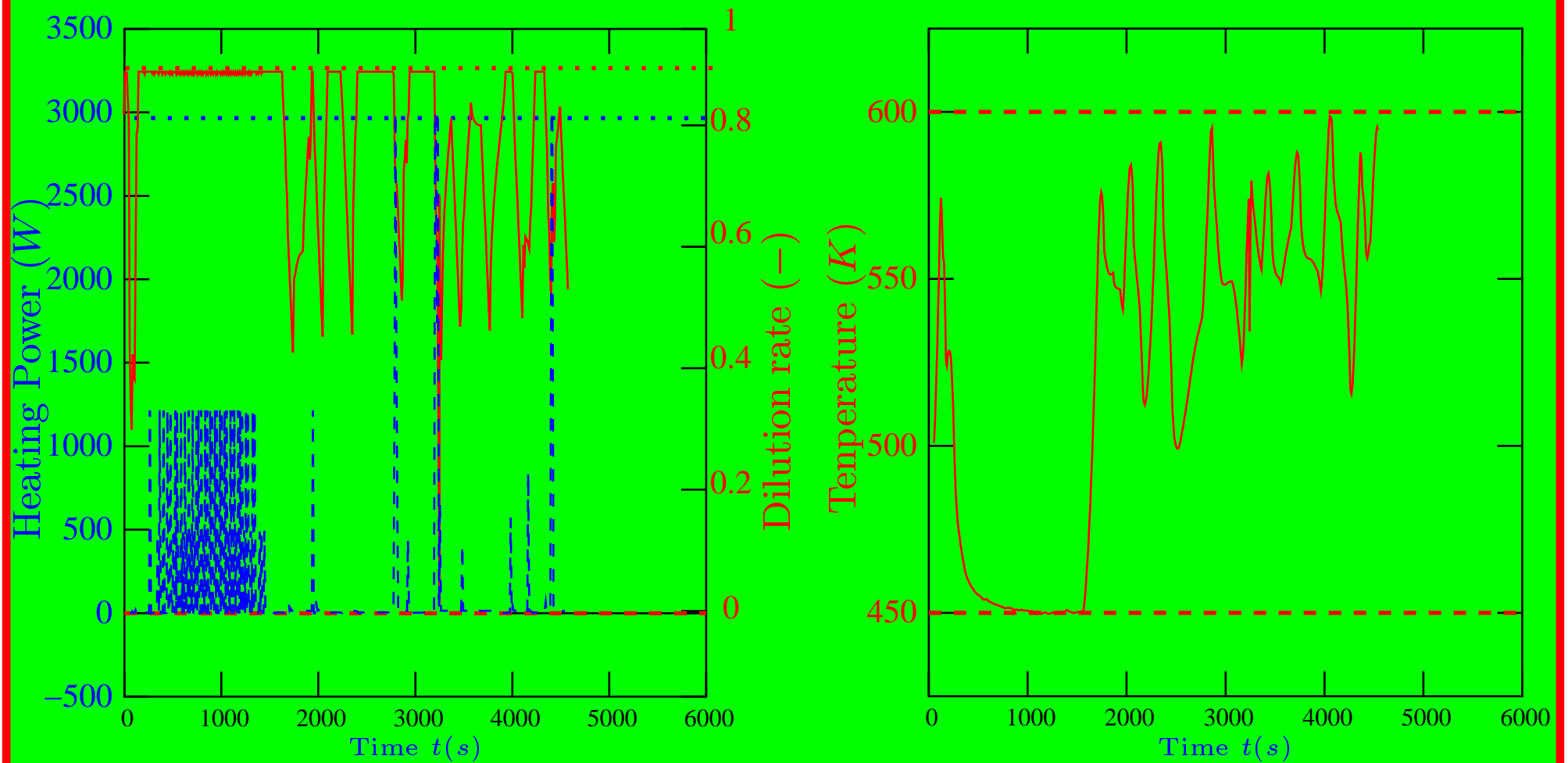
- The **dynamic of the temperature** involved in the output constraints is relatively **low** and has to be accounted for into the constrained optimization problem.

Conclusion: a sufficiently large final prediction horizon is required.

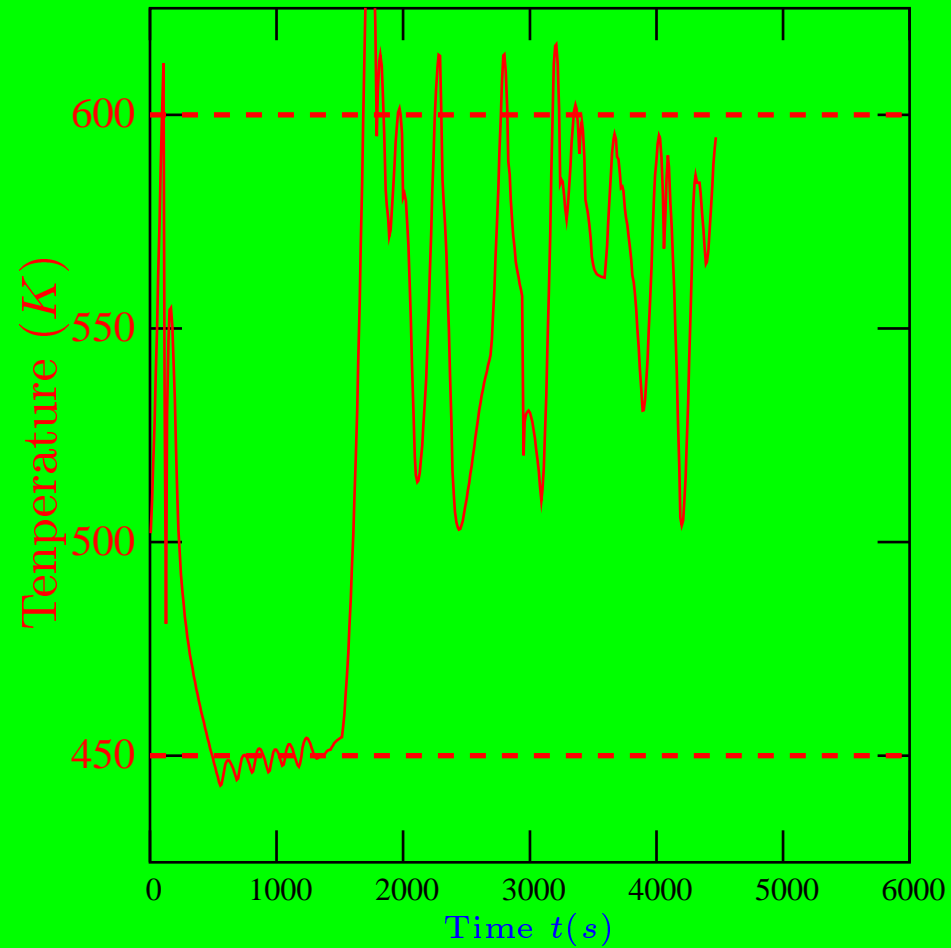
- Since ΔT_{ad} is used in the prediction framework, is strongly stochastic and has a large impact over closed-loop performances, **large prediction horizons will forecast an uncertain future.**

Conclusion: the smallest final prediction horizon is required.

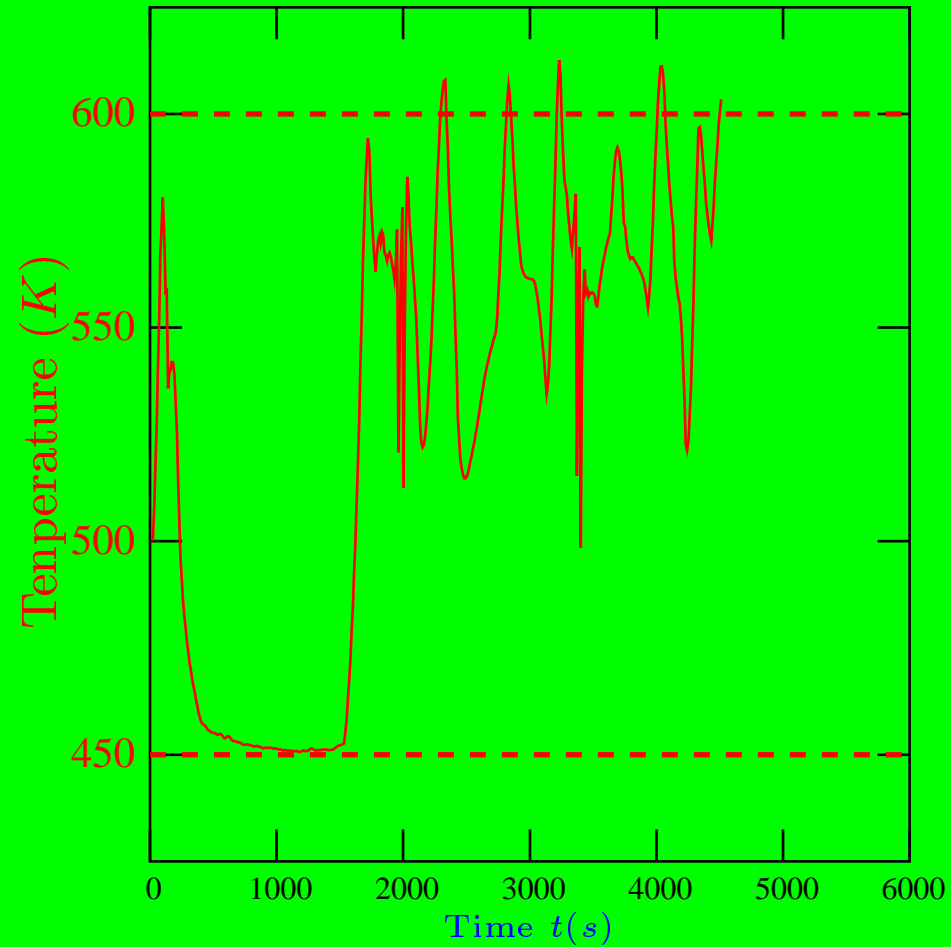
MPC: simulation #778, $hp_1^i = 2$, $hp_1^f = 4$, $hp_2^i = 1$, $hp_2^f = 12$



MPC: simulation #798 (= #778 w/o observer)



MPC: simulation #787, $hp_1^i = 1$, $hp_1^f = 3$, $hp_2^i = 8$, $hp_2^f = 8$



Conclusions

- In spite of the **input disturbance**, T_s can be **maintained** by both controllers **inside the specified temperature envelope**.
- Concerning the optimization performances, **LQR > MPC** since it requires **less heating action while treating more gas**: ($\bar{Q}_j = 83.4W$, $\bar{\alpha} = 0.894$) for LQR, ($\bar{Q}_j = 274.6W$, $\bar{\alpha} = 0.849$) for MPC ($0 \leq t \leq 4500s$). **MPC overevaluates** the real control needs since the stochastic variations of the input disturbance.
- With the non minimum phase behaviour of the process, the **horizons tuning is uneasy for the MPC**.
- A switching control structure is used for the LQR: therefore, heating and cooling action are initially decoupled. The drawback is that it introduces a severe **nonlinearity for stability analysis** whereas **MPC is more suitable than the LQR for general MIMO control problems**.

Thanks for your attention !



Notation

a_c = Specific solid-fluid surface area [m^{-1}]

c_{ps} = Solid heat capacity [$J.kg^{-1}.K^{-1}$]

c_{pmg} = Fluid heat capacity [$J.kg^{-1}.K^{-1}$]

H = Total length of monolith [m]

h = Solid-fluid heat transfer coefficient [$W.m^{-2}.K^{-1}$]

k_D = Solid-fluid mass transfer coefficient [$m.s^{-1}$]

M = VOC molecular weight [$kg.mol^{-1}$]

N' = Number of transfer units for heat loss [-]

P = Peclet number for solid-fluid heat transfer [-]

P_{ax} = Axial Peclet number for heat conduction [-]

P_θ = P corrected for the finite frequency [-]

Q_j = External power supply [W]

S = Total cross-section of the monolith [m^2]

T_{g1}, T_{g2} = Gas temperature in the upstream, downstream monolith [K]

Notation

T_0 = Inlet and external temperature [K]

T_{max} = Maximum solid temperature in the RFR [K]

T_s or T = Solid temperature [K]

t = Time [s]

u_{v0} = Superficial gas velocity in the reference state [$m.s^{-1}$]

x = Reduced abscissa, $2z/H$ [-]

z = Abscissa [m]

α = fraction of feed flow rate [-]

ΔH = Reaction enthalpy [$J.mol^{-1}$]

ΔT_{ad} = Adiabatic temperature rise [K]

ε = fraction of open frontal area [-]

$\varphi(x)$ = Characteristic function of the catalytic monolith [-]

$\psi(x) = \varphi(x)(\omega_1 + \omega_2)/(2\omega_{10})$ [-]

ρ = Fluid density [$kg.m^{-3}$]

Notation

ρ_0 = Gas density in the reference state [$kg.m^{-3}$]

ρ_s = Solid density [$kg.m^{-3}$]

τ = Heat storage time constant [s]

θ = Period of flow reversal [s]

$\omega_{1su}, \omega_{2su}$ = VOC mass fraction of solid phase in the up/downstream monoliths [-]

ω_1, ω_2 = VOC mass fraction in the up/downstream monoliths [-]

ω_{10} = VOC mass fraction in the feed [-]

ξ = Reduced abscissa of the boundary between inert/catalytic monoliths

ξ_θ = ξ corrected for the finite frequency [-]

X = State vector

X_e = Estimated state vector

y = Filtered temperature measurements [K]

Ω = Calibration parameter of the observer [-]

Gains in the LQR: algebraic Riccati equation

$$\left\{ \begin{array}{l} F^0 = (p_2^0)^{-1} (B_2^0)^T S^0 \\ S^0 A(\alpha^0) + (A(\alpha^0))^T S^0 + C^T C - S^0 B_2^0 (p_2^0)^{-1} (B_2^0)^T S^0 = 0 \\ F^1 = (p_2^1)^{-1} (B_1^1)^T S^1 \\ S^1 A(\alpha^1) + (A(\alpha^1))^T S^1 + C^T C - S^1 B_1^1 (p_2^1)^{-1} (B_1^1)^T S^1 = 0 \end{array} \right. \quad (3)$$

where $C = [C_1 \dots C_{100} \ C_{101} \dots C_{200}]$ with $[C_1 \dots C_{100}] = [0 \dots 0]$ and $[C_{101} \dots C_{200}] = [1 \ 0 \dots 0]$.

MPC: Constraints on the manipulated variable:

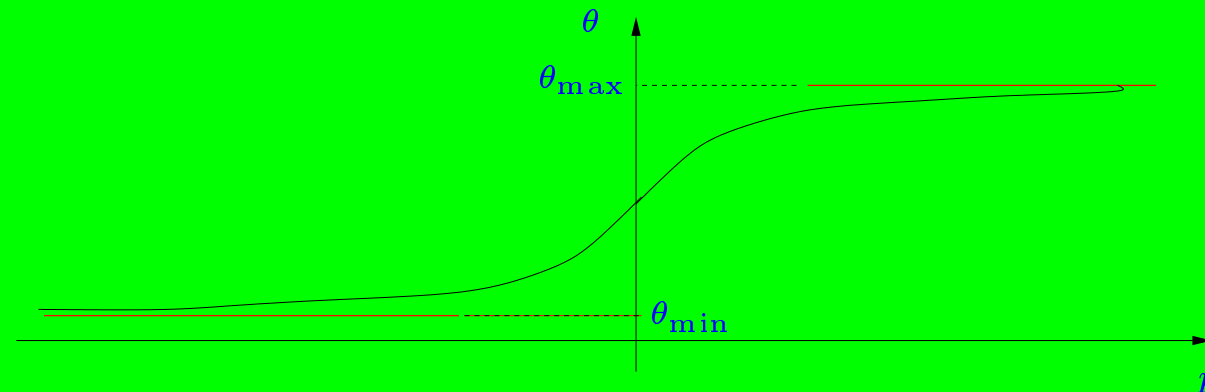
a transformation method [Fletcher, 1987]

From the **constrained variable** θ :

$$\theta_{\min} \leq \theta \leq \theta_{\max}$$

an **unconstrained variable** p is defined such that:

$$\theta = f(p) = \frac{1}{2}(\theta_{\max} + \theta_{\min}) + \frac{1}{2}(\theta_{\max} - \theta_{\min}) \tanh(p)$$



MPC: Constraints on measured and estimated variables:

external penalty method [Fletcher, 1987]

$$\min_{\beta} J_{tot}(\beta) = J(\beta) + w H(c_i(\beta)) \quad (i \in \mathcal{I})$$

$$\beta \in \mathbb{R}^{\beta}, w > 0$$

$$H(c_i(\beta)) = \sum h_i(c_i(\beta)) \quad \beta \in \mathcal{I}$$

here h_i is any C^1 function (at least) such that:

- $h_i(c_i(\beta)) = 0$ if $c_i(\beta) \leq 0$

(i.e. when the constraint is satisfied or saturated)

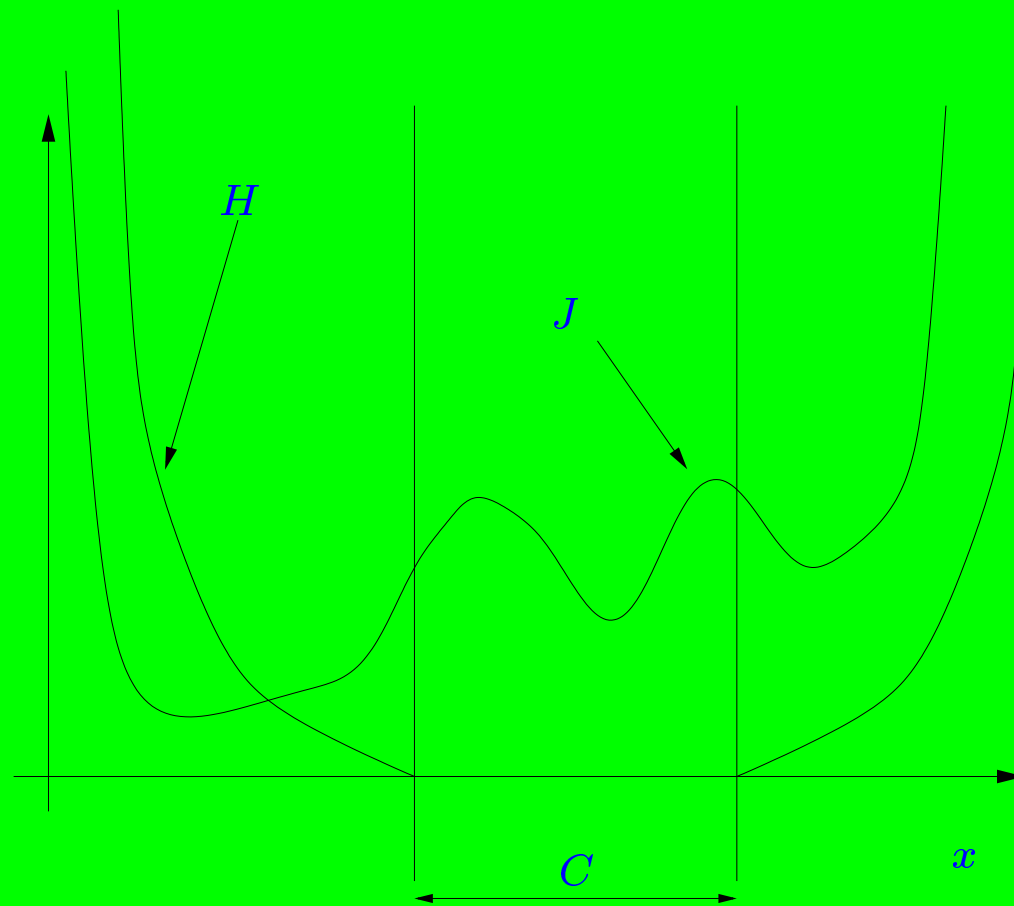
- and $h_i(c_i(\beta)) > 0$ if $c_i(\beta) > 0$

(i.e. when the constraint is not satisfied)

here: $h_i(c_i(\beta)) = \max^2(0, c_i(\beta))$

MPC: Constraints on measured and estimated variables:

external penalty method [Fletcher, 1987]



References (1)

- Budman, H., Kzyonsek, M. & Silverston, P. (1996). Control of a nonadiabatic packed bed reactor under periodic flow reversal. *Canadian J. of Chem. Eng.*, 74, 751-759.
- Cunill, F., Van de Beld, L. & Westerterp, K.R. (1997). Catalytic combustion of very lean mixtures in a reverse flow reactor using an internal electrical heater. *Ind. Eng. Chem. Res.*, 36, 4198-4206.
- Dufour, P., Couenne, F. & Touré, Y. (2003). Model predictive control of a catalytic reverse flow reactor. Special issue of *IEEE Trans. on Control Syst. Technol.* on Control of Industrial Spatially Distributed Parameter Processes, 11(5), 705-714.
- Dufour, P. & Touré, Y. (2004). Multivariable model predictive control of a catalytic reverser flow reactor. *Comput. & Chem. Eng.*, 28(11), pp. 2259-2270.

References (2)

- Edouard, D., Dufour, P. & Hammouri, H. (200?). Observer based multivariable control of a catalytic reverse flow reactor: comparison between LQR and MPC approaches. to be published in *Computers & Chemical Engineering*.
- Fletcher, R. (1987). *Practical methods of optimization*. John Wiley and Sons.
- Keith, J.M. (2003). Controlling reverse-flow reactors via multiscale transient thermal dispersion. *Adv. in Environm. Res.*, 7(2), 521-535.
- Nieken, U., Kolios, G. & Eigenberger, G. (1995). Limiting cases and approximate solutions for fixed-bed reactors with periodic flow reversal. *AIChE J.*, 41(8), 1915-1925.
- Ramdani, K., Pontier, R. & Schweich, D. (2001). Reverse low reactor at short switching periods for VOC combustion. *Chem. Eng. Sci.*, 56(4), 1531-1539.