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1

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Model Predictive Control of the Primary Drying Stage of the Drying of Solutions in Vials: an Application of the MPC@CB Software (Part 1)

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ADC'07, Hong Kong, August, 13-15 2007

Outline

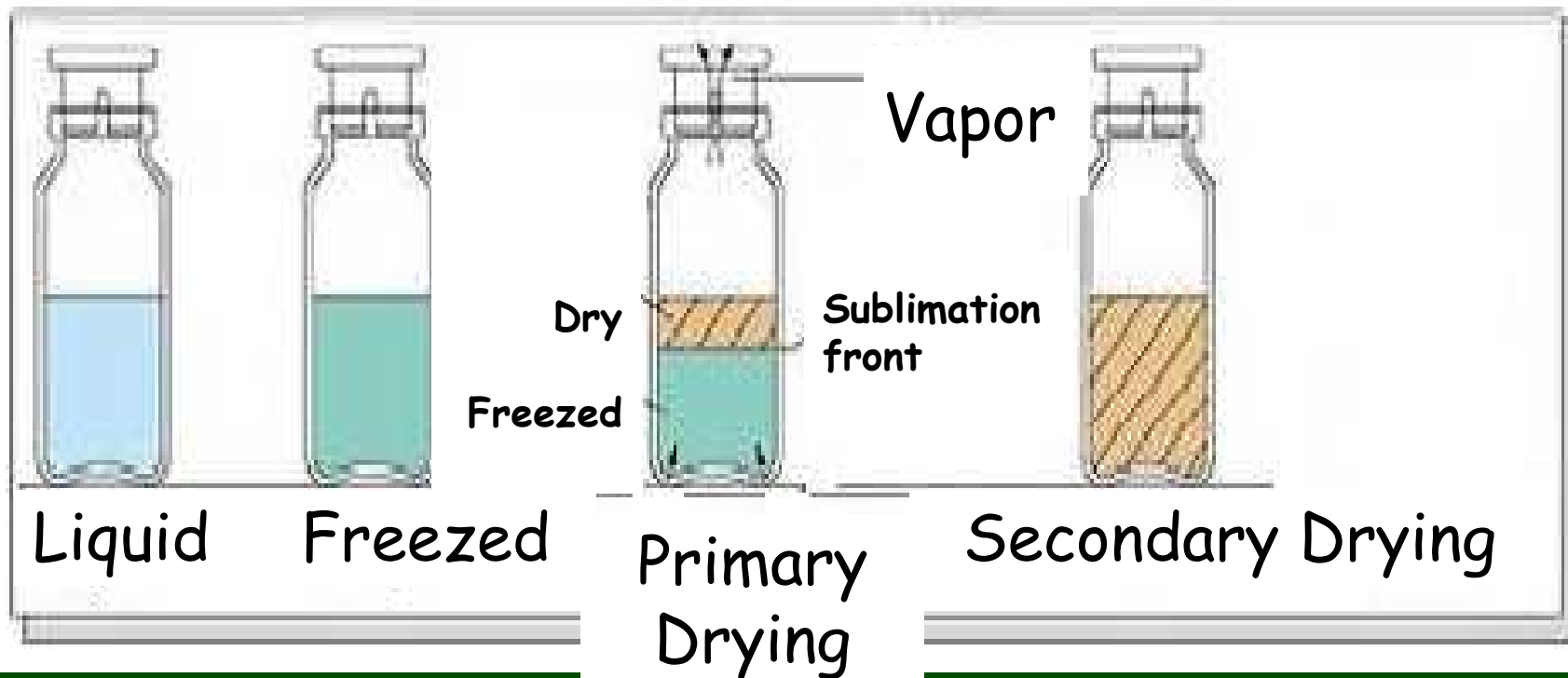
1. Control problem statement
2. First principle PDE model
3. Model predictive control strategy
4. MPC@CB© software main features
5. Simulation results
6. Conclusions & perspectives

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Control problem statement

- Freeze drying is generally considered to produce higher quality dried products.
- Here, freeze drying of solutions in vial must be controlled under constraints during the primary stage



Control problem statement *[Dufour, IDS06]*

- 1979: use of control tools in drying started.
- Since 1998: joined development of optimal control and first principle model in drying.
- Use of advanced control tools allows:
 - improving benefits,
 - decreasing energy use and off-spec production.
 - moreover, return on investment is relatively low.
- More first principle models are now needed !
- 60 000 products dried + 100 dryer types: a real potential of new collaborations between control and drying communities exist to improve dryer efficiency !

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First principle PDE model

- A **dynamic model** of the primary drying stage of the freeze drying process is needed: fundamental mass and energy balance equations are used.
- One dimensional **heat and mass transfer**.
- **Sublimation front** is planar and parallel to the horizontal section of the vial.
- Gas phase inside the pores of the dry layer is only composed of pure water vapor.
- Partial pressure of water vapor at the top of the dry layer = total pressure in the sublimation chamber.

First principle PDE model

T_1	Temperature in the dried layer	(K)
T_2	Temperature in the frozen layer	(K)
$H(t)$	Geometric shape of the moving interface	(m)
N_t	Total mass flux	(kg/m ² s)
ρ_{Ie}	effective density	60(kg/m ³)
c_{pI}	heat capacity	2590(J/kgK)
k_{Ie}	thermal conductivity	
c_{pg}	specific heat capacity at constant pressure	1616.16(J/kg)
M_w	Molecular weight of water vapor	18.10 ⁽⁻³⁾ (kg/mol)
ϵ	void fraction of dried layer	
R_{ig}	ideal gas constant	8.314(Pam ³ /Kmol)
T^o	temperature at $t = 0$	230.15(K)
p_w^o	partial pressure at $t = 0$	8(N/m ²)
k_{II}	thermal conductivity	2.1(W/Km)
α_2	thermal diffusivity	
σ	Stefan-Boltzman constant	5.6710 ⁽⁻⁸⁾ (W/m ² K)
F_{up}	view factor for radiative heat transfer	0.795
h_v	heat transfer coefficient	30(W/Km ²)
k_1	bulk diffusivity constant	0.001
$f(T_z)$	water vapor pressure at the moving interface	$exp(-6320.1517/T + 29.5578)$
ΔH_s	heat of sublimation of ice	248010 ⁽⁻³⁾ (J/kg)

State variables

TAB. 1 – Parameter values and expressions

First principle PDE model

[Liapis et al., 1994]

Dynamic equations:

$$\left\{ \begin{array}{l} \rho_{Ie} c_{pI} \frac{\partial T_1}{\partial t} = k_{Ie} \frac{\partial^2 T_1}{\partial z^2} - c_{pg} \frac{\partial(N_t T_1)}{\partial z} \quad t > 0, \quad 0 < z < Z = H(t) \\ \frac{\partial T_2}{\partial t} = \alpha_2 \frac{\partial^2 T_2}{\partial z^2}, \quad t > 0, \quad H(t) < z < L \\ \frac{\partial H}{\partial t} = -\frac{N_t}{(\rho_{II} - \rho_I)} \quad t > 0, \end{array} \right.$$

$$N_t = N_w = -\frac{M_w k_1}{R_{ig} T_1 |_{z=H(t)} H(t)} (p_{wH} - p_w^o) \quad t > 0$$

First principle PDE model

[Liapis et al., 1994]

Boundary conditions:

Control variables

$$\left\{ \begin{array}{l} -k_{Ie} \frac{\partial T_1}{\partial z} \Big|_{z=0} = \sigma F_{up} (T_{up}^4 - T_1^4 \Big|_{z=0}), \quad t > 0, \quad z = 0 \\ k_{II} \frac{\partial T_2}{\partial z} - k_{Ie} \frac{\partial T_1}{\partial z} + \frac{dH(t)}{dt} (\rho_{II} c_{pII} T_2 - \rho_I c_{pI} T_1) = -\Delta H_s N_t \quad z = H(t) \\ k_{II} \frac{\partial T_2}{\partial z} \Big|_{z=L} = h_v (T_{lp} - T_2 \Big|_{z=L}) \quad t > 0 \quad z = L \end{array} \right.$$

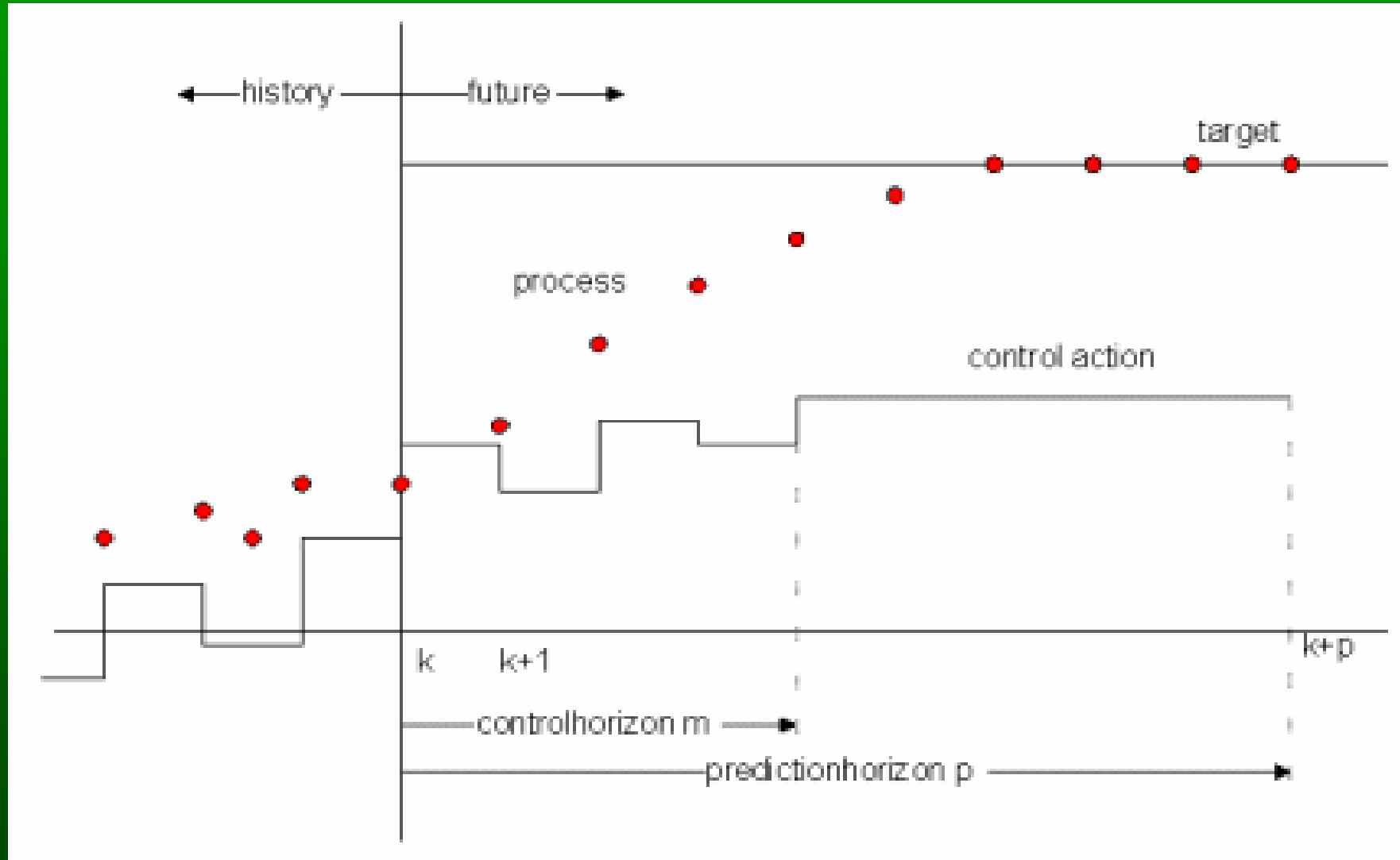
Initial conditions:

$$T_1(z, t) = T_2(z, t) = T^0, \quad t > 0, \quad 0 < z < L$$

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Model predictive control strategy



Model predictive control strategy

$$\min_u J(u) = \sum_{j=k+1}^{j=k+N_p} [f(y_{ref}(j), y_p(j))]$$

subject to constraints on the manipulated variable :

$$u_{min} \leq u(j) \leq u_{max} \forall j \in \{k+1, k+N_p\}$$
$$\Delta u_{min} \leq u(j) - u(j-1) \leq \Delta u_{max} \forall j \in \{k+1, k+N_p\}$$

subject to constraints on the controlled variable :

$$c(y_p(j), y_{ref}(j)) \leq 0 \forall j \in \{k+1, k+N_p\}$$

The function f means: trajectory tracking, processing time minimization, productivity function ...

Model predictive control strategy

Advantages:

- **constraints** (such as manipulated variables physical limitations, constraints due to operating procedures or safety reasons...) may be specified
- a model aims to **predict** the future behavior of the process and the best one is chosen by a correct **optimal control** of the manipulated variables.

Drawbacks:

- **computational time** needed may limit online use
- **suboptimal solutions**
- **how to handle unfeasibilities**

Model predictive control strategy

[Dufour et al, IEEE TCST 11(5) 2003]

- Originally developed for nonlinear PDE model control
- Main idea: decrease the online time needed to compute the PDE model based control

Approach:

- Input constraints: hyperbolic transformation
- Output constraints: exterior penalty method
- Linearization + sensitivities computed off line
- On line use of a time varying linear model
- On line resolution of a penalized (and so unconstrained) optimization control problem : a modified Levenberg Marquardt Algorithm

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MPC@CB© software main features

1. Developed under Matlab, MPC@CB© solves any user defined :
 - trajectory tracking problem
 - operating time minimization problem
 - any cost function
 - input/output constraint handled
2. Any user defined continuous model (SISO, MISO, SIMO, MIMO model), including large scale PDE model
3. Easy to introduce a user defined observer
4. Easy to apply the software for simulation or real time application

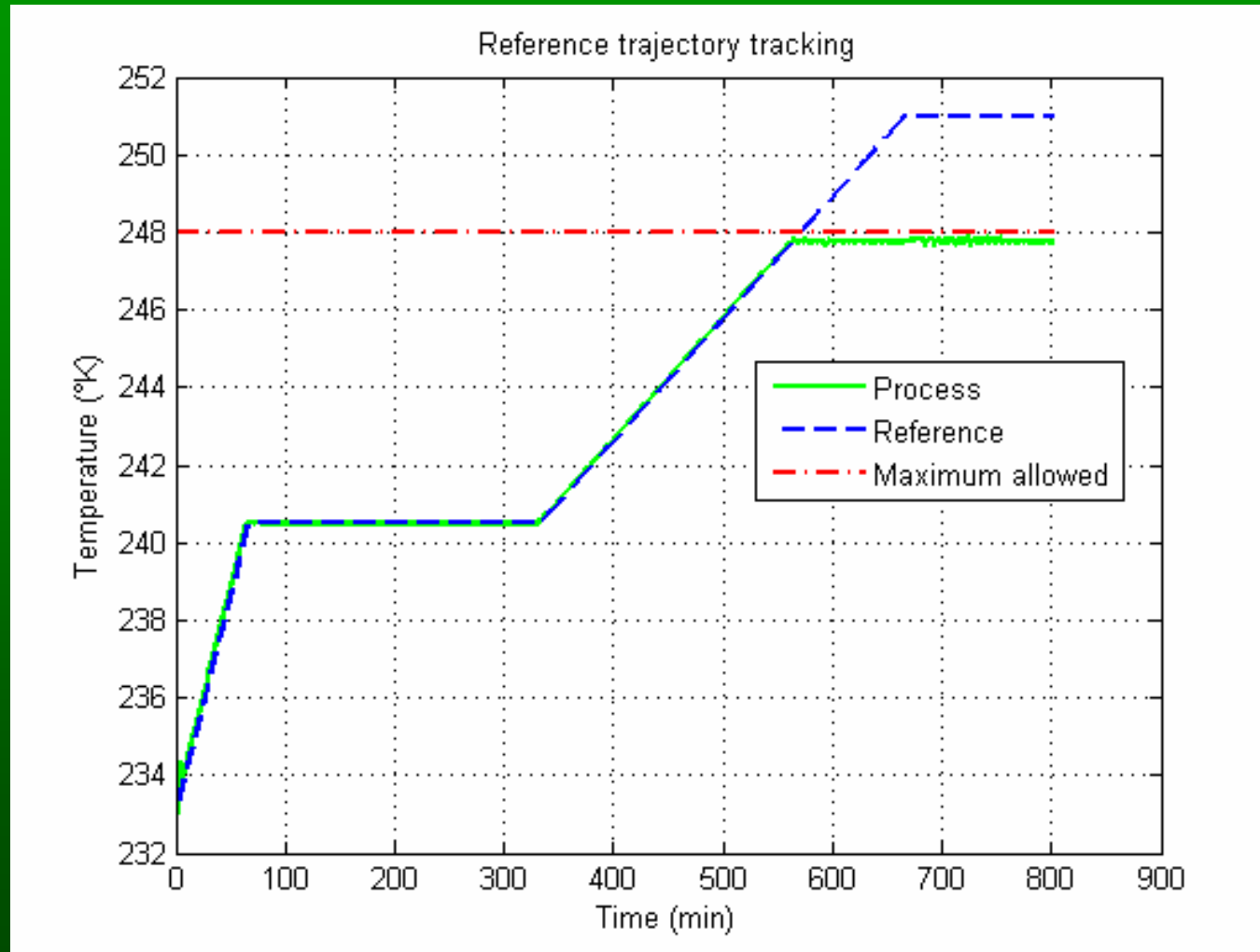
MPC@CB ©: flexibility/ease for a quick use in control !

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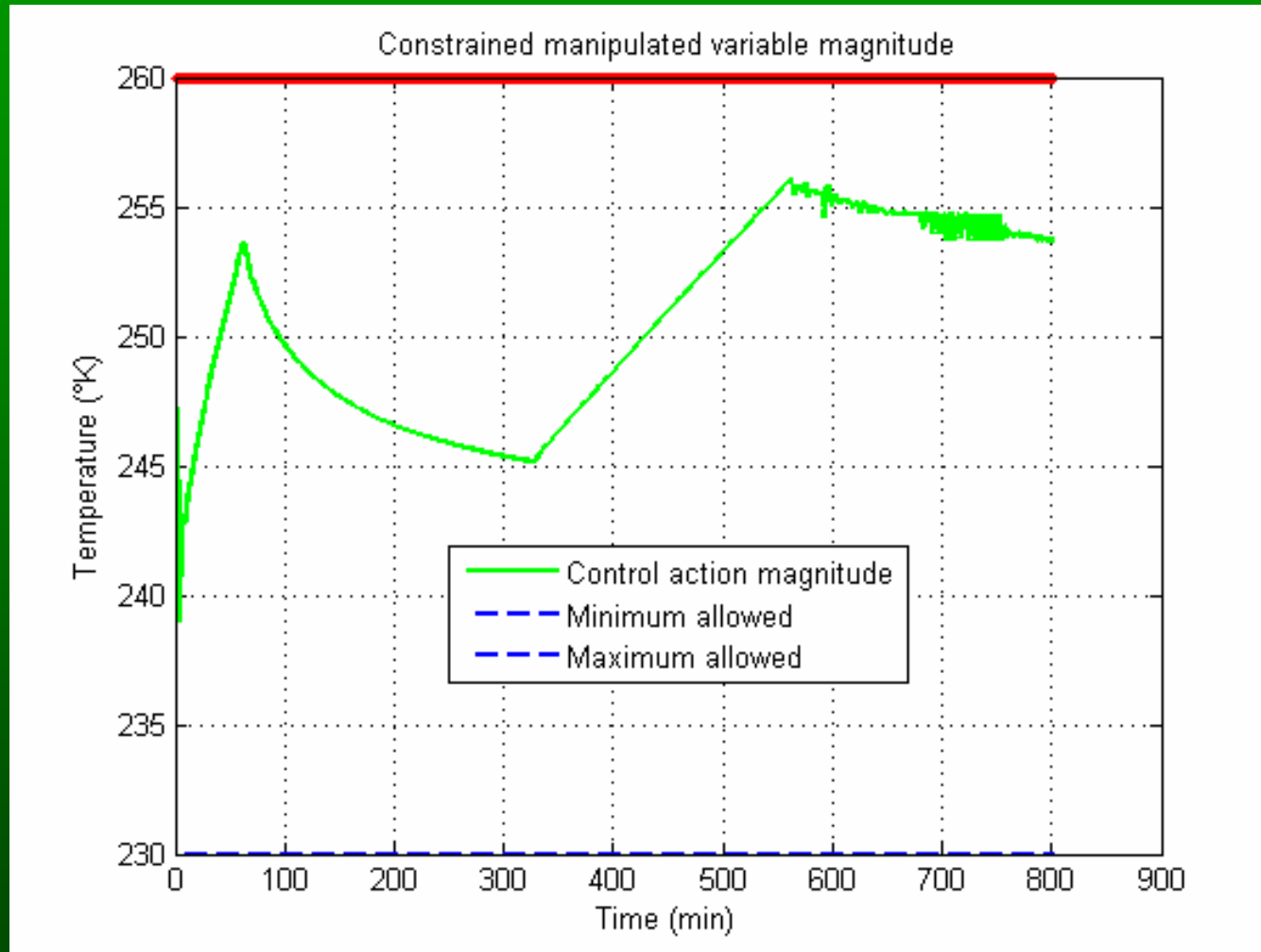
Simulation results

Temperature trajectory tracking with magnitude+velocity input constraints+ output constraint



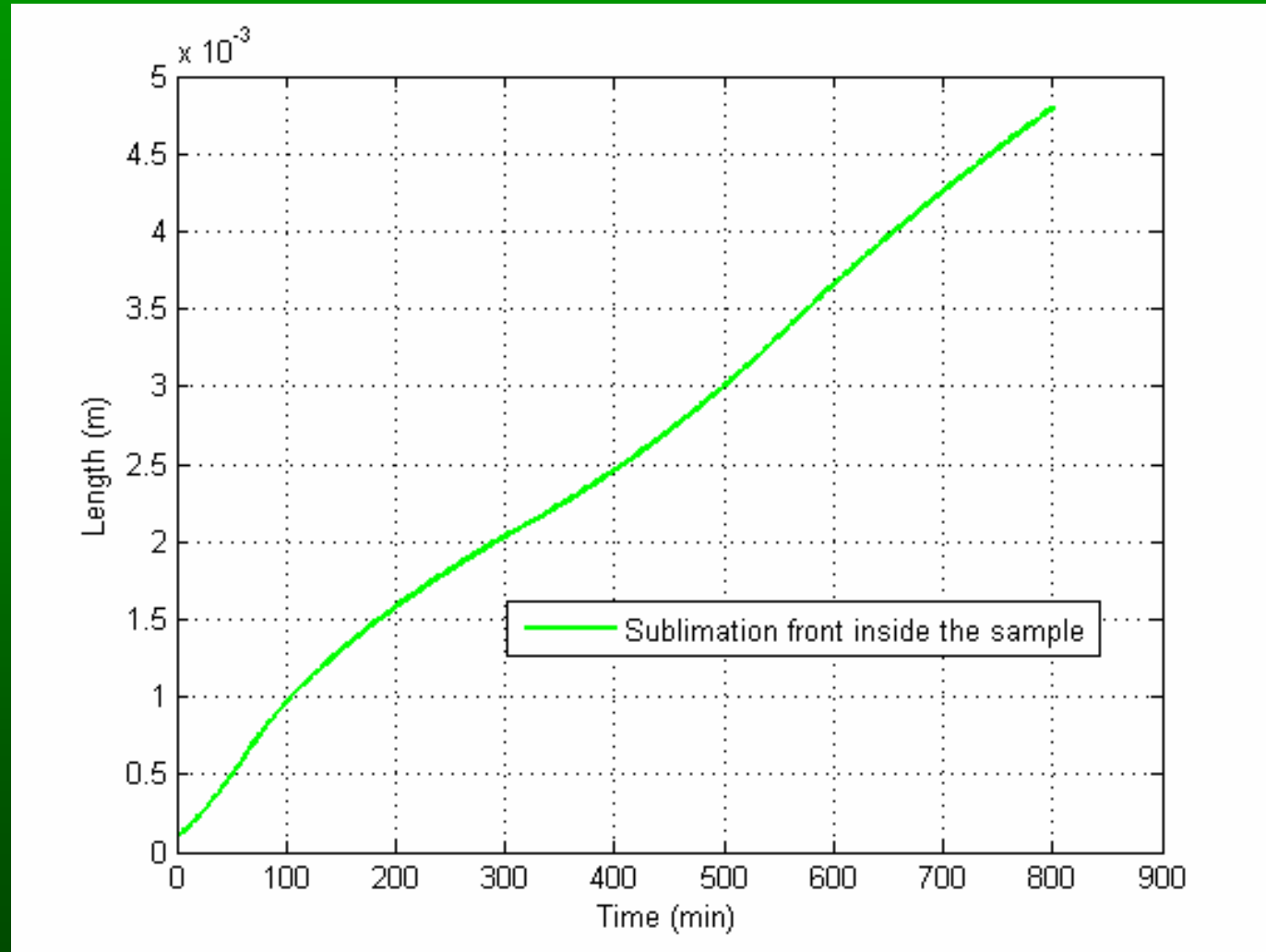
Simulation results

Temperature trajectory tracking with magnitude+velocity input constraints+ output constraint



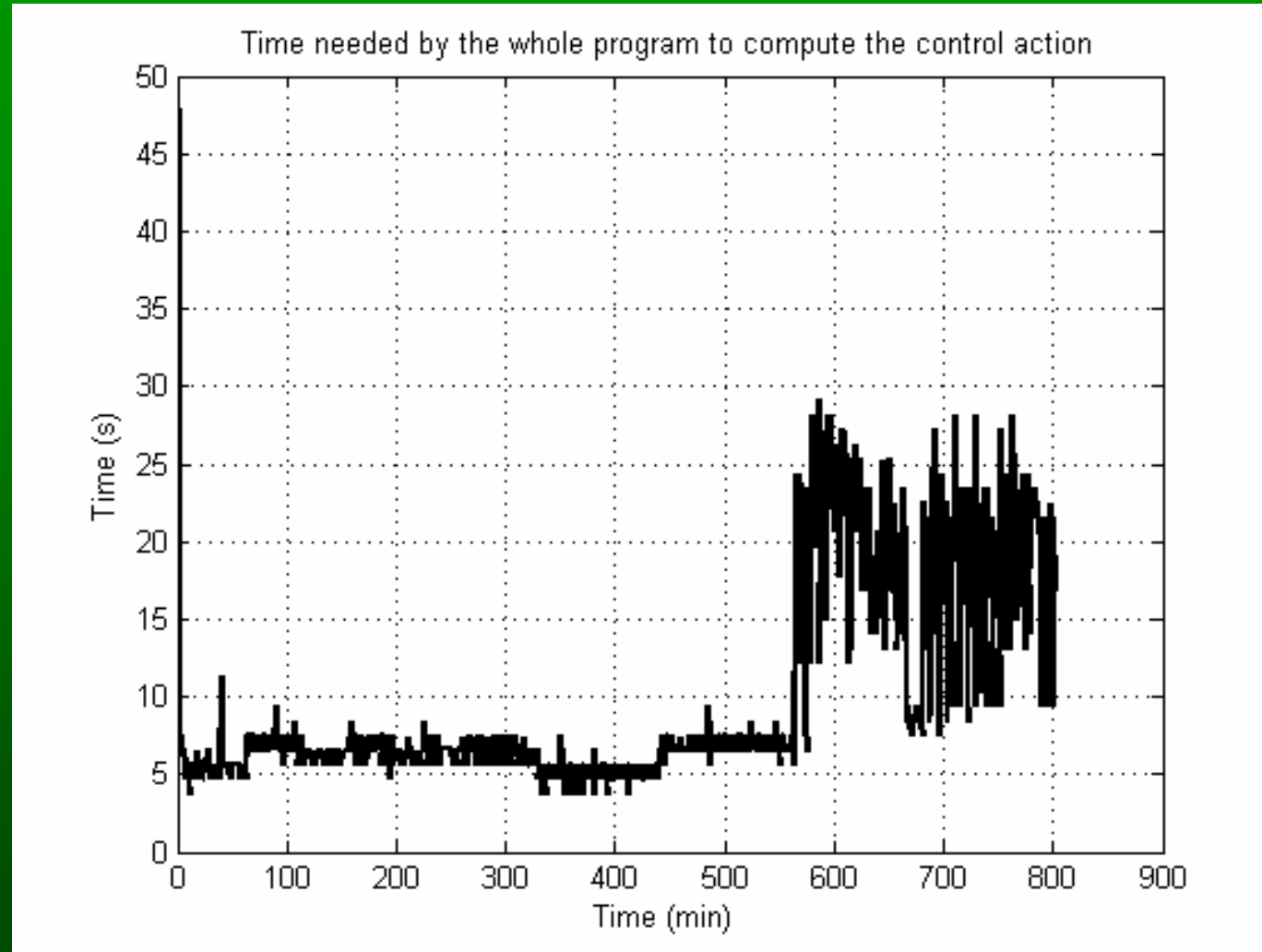
Simulation results

Temperature trajectory tracking with magnitude+velocity input constraints+ output constraint



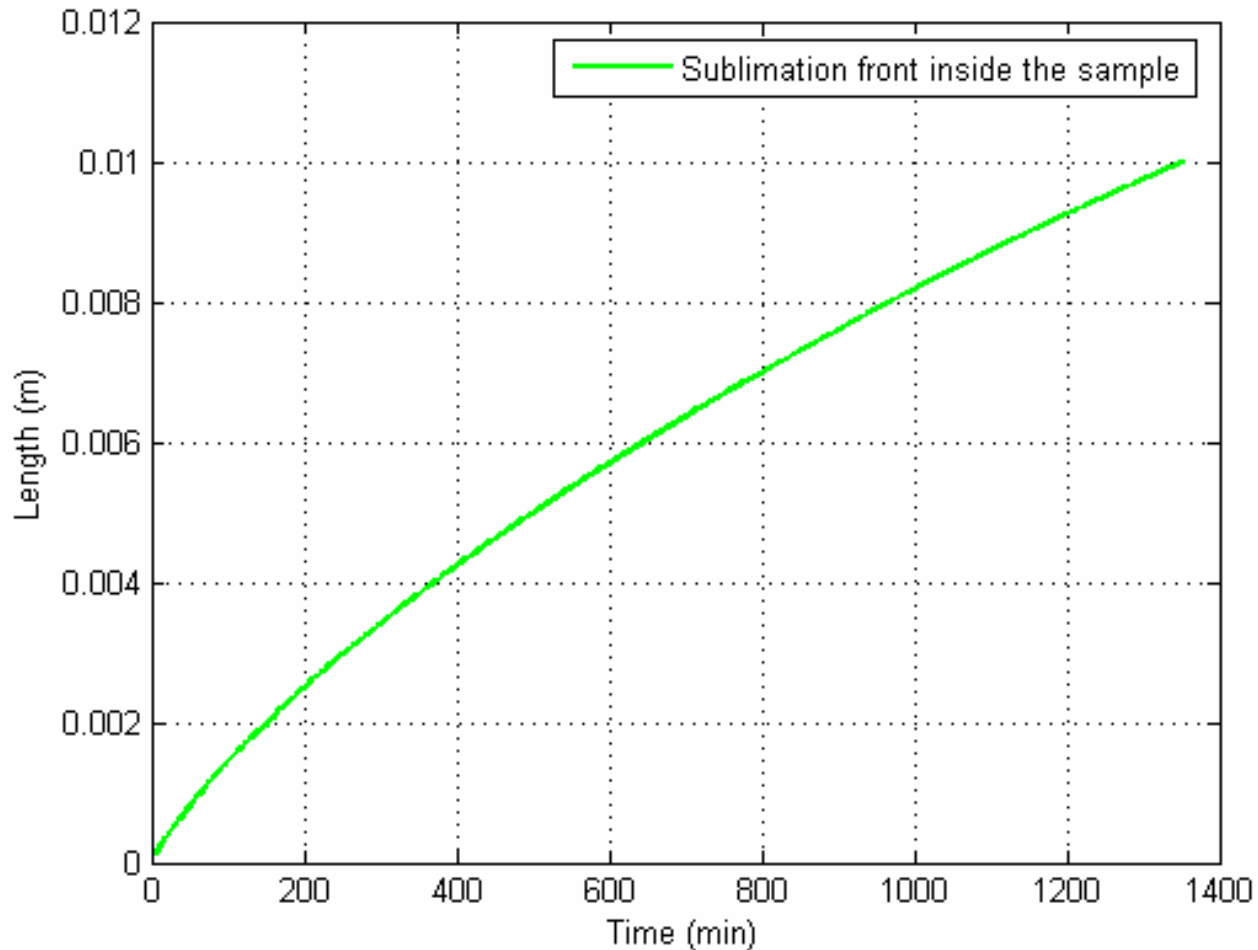
Simulation results

Temperature trajectory tracking with magnitude+velocity input constraints+ output constraint (sampling time=60s)



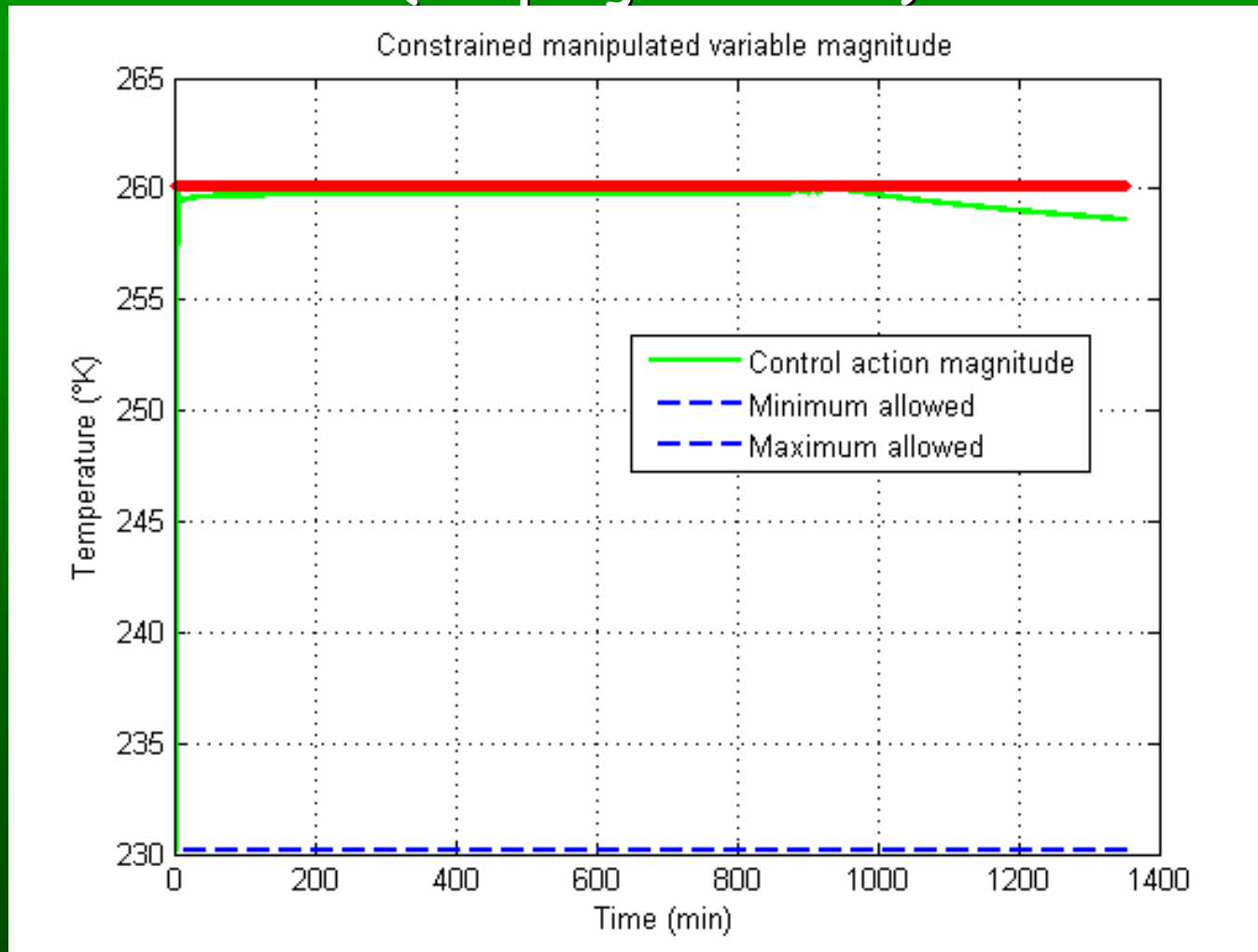
Simulation results

Maximization of the sublimation front velocity with magnitude+velocity input constraints + output constraint (sample size=1 cm)



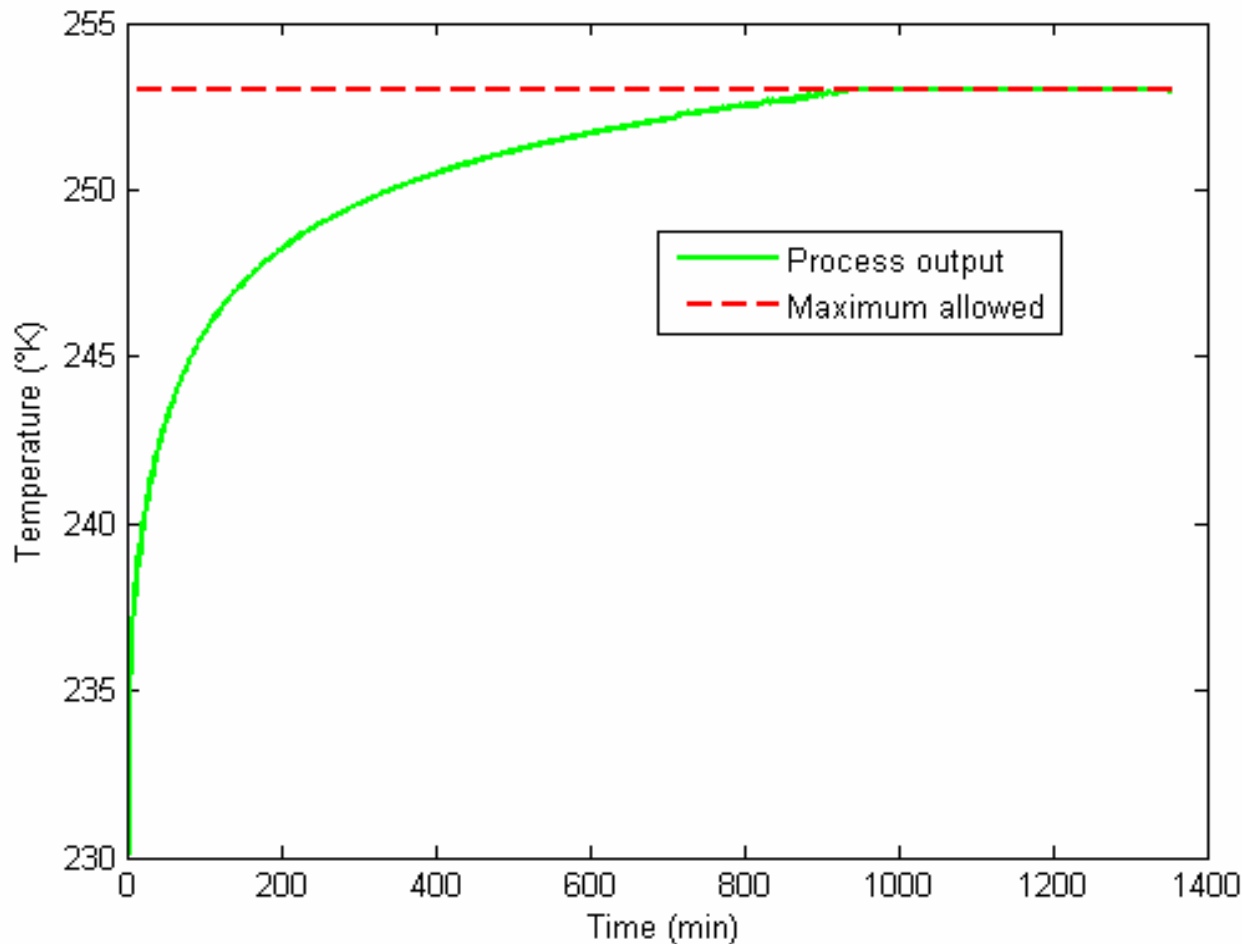
Simulation results

Maximization of the sublimation front velocity with magnitude+velocity input constraints + output constraint (sampling time=60s)



Simulation results

Maximization of the sublimation front velocity with magnitude+velocity input constraints + output constraint (sampling time=60s)



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Conclusions

- The real time control of drying of vials is possible
- Control of such system by a general MPC@CB© software has been shown

Perspectives

- Experimental validation
- Experimental minimization of the drying time under constraints: an observer (model based soft sensor) is under development
- MPC@CB© may be used for any process: since its development, it is also currently used for control of polymer production, painting curing, pasta drying.
- To use MPC@CB©: dufour@lagep.univ-lyon1.fr



Thank you



Any questions ?



First principle PDE model

[Liapis et al., 1994]

Need for a change of space coordinates:

$$\xi_1 = \frac{z}{H(t)}, \quad \xi_2 = \frac{H(t) - z}{H(t) - L}$$

$$\begin{aligned} \tilde{T}_1(\xi_1, t) &= T_1(z, t) \\ \tilde{T}_2(\xi_2, t) &= T_2(z, t) \end{aligned}$$

Then, space and time derivative operators becomes:

$$\begin{aligned} \frac{\partial T_1}{\partial z} &= \frac{1}{H(t)} \frac{\partial \tilde{T}_1}{\partial \xi_1}, \quad \frac{\partial^2 T_1}{\partial z^2} = \frac{1}{H^2(t)} \frac{\partial^2 \tilde{T}_1}{\partial \xi_1^2}, \quad \frac{\partial T_1}{\partial t} = \frac{\partial \tilde{T}_1}{\partial t} - \frac{\dot{H}(t)}{H(t)} \frac{\partial \tilde{T}_1}{\partial \xi_1} \xi_1 \\ \frac{\partial T_2}{\partial z} &= \frac{-1}{(H(t) - L)} \frac{\partial \tilde{T}_2}{\partial \xi_2}, \quad \frac{\partial^2 T_2}{\partial z^2} = \frac{1}{(H(t) - L)^2} \frac{\partial^2 \tilde{T}_2}{\partial \xi_2^2}, \quad \frac{\partial T_2}{\partial t} = \frac{\partial \tilde{T}_2}{\partial t} + \frac{(1 - \xi_2)\dot{H}(t)}{(H(t) - L)} \frac{\partial \tilde{T}_2}{\partial \xi_2} \end{aligned}$$

First principle PDE model

[Liapis et al., 1994]

The PDE model with boundary control is:

$$\left\{ \begin{array}{ll} \frac{\partial X_m}{\partial t} = F_d(X_m) & 0 < \xi_1 < 1, 0 < \xi_2 < 1, t > 0 \\ F_b(X_m, u) = 0 & \xi_1 \in \{0, 1\}, \xi_2 \in \{0, 1\}, t > 0 \\ Y_m = CX_m & \xi_2 = 1, t > 0 \\ X_m(\xi_1, \xi_2, 0) = X^0(\xi_1, \xi_2) & \end{array} \right.$$