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Lyapunov exponents with Model Predictive Control for exothermic batch reactors

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Abstract: Thermal runaways cause significant safety issues and financial loss for industrial batch reactors due to the disruption of normal operation. The intensification of processes is restricted, since control systems are not capable of detecting stability boundaries of the system and hence are overly conservative. For this purpose Lyapunov exponents are introduced as a stability criterion. It is shown that Lyapunov exponents can correctly predict the stability of batch reactor systems. This stability criterion is embedded in Model Predictive Control, which results in a novel control scheme. This scheme allows the controlled increase of the reaction temperature to achieve a target conversion in a reduced completion time of reaction.

Keywords: Process and Control Monitoring, Batch Process Modelling and Control, Process Intensification

1. INTRODUCTION

Batch processes are very important for the chemical industry, since a vast amount of speciality chemicals is produced in this reactor type. One advantage of using batch or semi-batch reactors, as opposed to continuous reactors, is the flexibility in process strategy and control, due to the possibility to control an additional input. This involves processes operating in non-steady state operation, which are harder to control.

Thermal runaways occur when the heat generated by exothermic reactions exceeds the cooling capacity of the reactor, ultimately resulting in an explosion. Stability criteria which reliably predict how close the system is to instability are therefore of major interest for the industry.

Many criteria can been found in literature which describe system stability. The first stability criterion was developed by Semenov, who introduced the Thermal Explosion Theory (Semenov, 1942). Introduction of many other stability criteria followed (Barkelew, 1959) which, including the Thermal Explosion Theory, gave bounds of steady-state operating points.

For dynamic systems one very common criterion is the Routh-Hurwitz criterion (Anagnost and Desoer, 1991). This criterion only reliably describes the stability of systems at steady-state. For non steady-state systems this criterion becomes unreliable.

The divergence criterion quantifies how much the variables are ‘diverging’ from each other based on the underlying system equations. This definition comes from chaos theory (Arnold, 1973), but is not very reliable for non steady-state systems and will therefore not be considered further.

Lyapunov exponents (Strozzi and Zaldvar, 1994) were later introduced to measure the stability of nonlinear systems using concepts from chaos theory. As will be shown, this criterion gives more reliable results for non steady-state systems, but can impose high computational cost.

In batch processes the heat generation of exothermic reactions decreases as the reagents are consumed. A time-dependent increase in reaction temperature in the stable region leads to an intensification of the process. The ability to detect instability of the process is of major importance for the control of such systems. Furthermore, a reliable measure of stability can improve operator knowledge greatly, and therefore vastly reduce the risk of thermal runaways occurring in industry. This has an important safety implication and decreases financial loss.

Model Predictive Control (MPC) is an advanced control scheme which optimises the control variables of the system, while considering system constraints. In literature most MPC schemes implement a linearisation of the system present, which can be used with a linear MPC scheme (Rawlings and Mayne, 2015). With such a formulation the stability of the closed-loop system can be proven theoretically by the use of Lyapunov functions (DeHaan and Guay, 2010). If no Lyapunov function can be found, end-point constraints are often employed. For complex and highly nonlinear systems this leads to higher computational cost as the system has to be simulated for a larger time frame. The use of an online stability criterion can reduce the time frame used by giving an indication of the system stability at each point of the simulation.

This work introduces a stability criterion based on Lyapunov exponents in a novel way, such that it can be integrated in Model Predictive Control algorithms in a seamless manner. Case studies demonstrate the efficacy of the approach and the enhanced performance gained over more traditional PI control systems and MPC algorithms without such embedded stability criteria.

2. BATCH REACTOR SYSTEM

In the model used for the subsequent simulations of batch processes, *i.e.* with constant volume, an irreversible, exothermic reaction is analysed which is given by:

$$\mathrm{A+B} \rightarrow \mathrm{C} \tag{1}$$

The model of the batch processes is based on differential equations for mass and energy balances. The reaction kinetics mainly consider component A, which are assumed to follow the Arrhenius equation (Davis and Davis, 2003). Examples of reactions with this kinetic scheme are polycondensation reactions, e.g. of dicarboxylic acid and diols, or the addition reaction for the synthesis of ethylene glycol from ethylene oxide and water. A diagram of the batch reactor system used is shown in Figure 1.

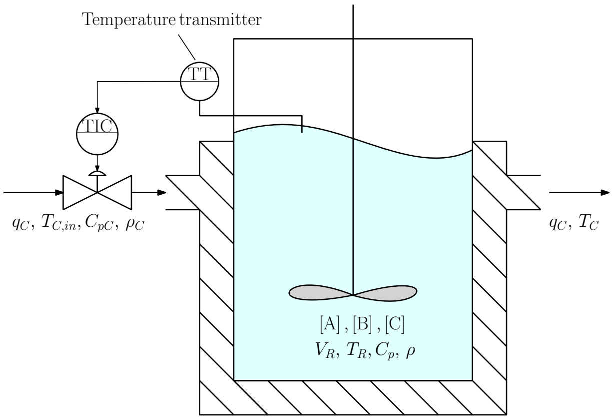

Fig. 1. Diagram of batch reactor with cooling jacket used for simulations.

The mass balances for each reagent and product are:

$$\frac{\mathrm{d}\,[\mathrm{A}]}{\mathrm{d}t} = -r\left([\mathrm{A}]\,,\, T_R\right) \tag{2}$$

$$\frac{\mathrm{d}\,[\mathrm{B}]}{\mathrm{d}t} = -r\left([\mathrm{A}]\,,\, T_R\right) \tag{3}$$

$$\frac{\mathrm{d}\,[\mathrm{C}]}{\mathrm{d}t} = +r\left([\mathrm{A}]\,,\, T_R\right) \tag{4}$$

$$r\left([\mathrm{A}]\,,\, T_R\right) = k_0\ [\mathrm{A}]^n\ \exp\left(-\frac{E_a}{R\,T_R}\right) \tag{5}$$

where [A], [B] and [C] are the concentrations of components A, B and C, t is time, r is the reaction rate, T_R is the reactor temperature, k_0 is the Arrhenius pre-exponential constant, n is the order of reaction with respect to component A, which is set to $n = 2$, E_a is the activation energy, and R is the universal molar gas constant. The energy balance for the reactor contents is given by:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(V_R\,\rho\,C_p\,T_R\right) = r\left([\mathrm{A}]\,,\, T_R\right)\ (-\Delta H_r)\ V_R \\ -U\ A\ (T_R - T_C) \tag{6}$$

where V_R is the reactor volume, ρ is the reactor content density, C_p is the heat capacity of the reactor contents, ΔH_r is the enthalpy of the reaction, U is the heat transfer coefficient and A is the heat transfer area.

A liquid, homogeneous reaction medium is modelled, which is why the physical properties and the volume of the reaction mixture are assumed to be constant. This leads to the following equation:

$$V_R\,\rho\,C_p \frac{\mathrm{d}}{\mathrm{d}t}\left(T_R\right) = r\left([\mathrm{A}]\,,\, T_R\right)\ (-\Delta H_r)\ V_R \\ -U\ A\ (T_R - T_C) \tag{7}$$

The energy balance for the cooling jacket is given by:

$$V_C\,\rho_C\,C_{pC} \frac{\mathrm{d}}{\mathrm{d}t}\left(T_C\right) = q_C\,\rho_C\,C_{pC}\,(T_{C,in} - T_C) \\ +U\ A\ (T_R - T_C) \tag{8}$$

where V_C is the cooling jacket volume, ρ_C is the coolant density, C_{pC} is the heat capacity of the coolant, $T_{C,in}$ and T_C are the coolant inlet and cooling jacket temperature and q_C is the volumetric coolant flow.

The physical properties of the reaction mixture and of the reactor used in the simulations are shown in Table 1.

Table 1. Process parameters for batch reactor simulations.

Parameter	Value
V_R	16 m^3
V_c	1.2 m^3
A	30.7 m^2
$T_{C,\,in}$	300 K
E_a/R	9525 K
k_0	$2.2\times10^5\ \mathrm{m^3\,kmol^{-1}\,s^{-1}}$
$q_{c,\,max}$	$0.037\ \mathrm{m^3\,s^{-1}}$
ρ	$1100\ \mathrm{kg\ m^{-3}}$
C_p	$2330\ \mathrm{J\ kg^{-1}\,K^{-1}}$
ρ_C	$1000\ \mathrm{kg\ m^{-3}}$
C_{pC}	$4180\ \mathrm{J\ kg^{-1}\,K^{-1}}$
U	$600\ \mathrm{W\ m^{-2}\,K^{-1}}$
ΔH_r	$-75\ \times10^6\mathrm{J\,kmol^{-1}}$
$[\mathrm{A}]_0$	$13\ \mathrm{kmol\ m^{-3}}$
R	$8.314\ \mathrm{mol\ J^{-1}\,K^{-1}}$

All simulations shown in this paper were carried out on a Dell XPS 13 with an Intel® Core™ i7-6560U processor, with operating system Windows 10 Home. The system dynamics were simulated using *ode15s* (Shampine et al., 1999) within MATLAB™.

3. LYAPUNOV EXPONENTS

The Lyapunov exponents describe how state variables "drift off" after a large amount of time for an initial small perturbation, ϵ. The deviation of the state variables is assumed to follow an exponential profile, which enables to quantify if a stable system is present. A diagram showing the evolution of this deviation is shown in Figure 2.

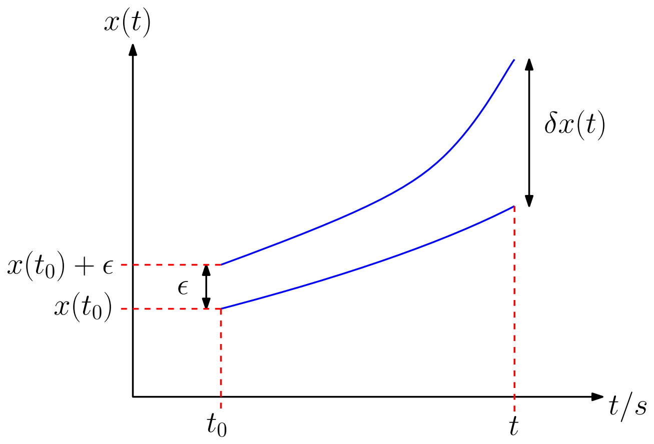

Fig. 2. Deviation of an initially perturbed state variable. In this case an unstable system is shown.

The following expression quantifies the deviation of an initially perturbed state variable after time t:

$$\epsilon \exp\left(\Lambda\left(x_0\right)t\right) = \left|x\left(t,\, x_0\right) - x\left(t,\, x_0+\epsilon\right)\right| \tag{9}$$

$$\Lambda\left(x_0\right) = \frac{1}{t}\ln\left(\frac{\left|x\left(t,\, x_0\right) - x\left(t,\, x_0+\epsilon\right)\right|}{\epsilon}\right) \tag{10}$$

At the limit of a very small perturbation and infinite time:

$$\Lambda\left(x_0\right) = \lim_{t\to\infty}\frac{1}{t}\ln\left(\left|\frac{\delta x\left(t,\, x_0\right)}{\delta x_0}\right|\right) \tag{11}$$

This is known as the *Lyapunov exponent* (Strozzi and Zaldvar, 1994). Numerically, Lyapunov exponents can be evaluated by simulating several systems in parallel, for which each state variable is perturbed initially by an amount $\epsilon = \delta x_0$. Simulating the systems for an infinite amount of time is of course infeasible. Therefore a large time horizon is chosen instead, which is supposed to give a good approximation of the final value, known as the local Lyapunov exponent. This means that at each point in time, a long simulation has to be carried out in order to find the local Lyapunov exponent, given by:

$$\Lambda_1\left(x_0\right) = \frac{1}{t_f}\ln\left(\left|\frac{\delta x\left(t_f,\, x_0\right)}{\delta x_0}\right|\right) \tag{12}$$

The time t_f in (12) is set in order to give a large time frame, which approximates the infinite horizon from the original definition. Other methods for evaluating the Lyapunov exponents are available (Melcher, 2003).

Due to the heat generation and removal of the reaction the variables of interest are [A], T_R and T_C. Hence, the local Lyapunov exponents for these variables are evaluated by:

$$\Lambda_{1,1} = \frac{1}{t_f}\ln\left(\left|\frac{[\mathrm{A}]\left(t_f, [\mathrm{A}]_0\right) - [\mathrm{A}]\left(t_f, [\mathrm{A}]_0+\epsilon\right)}{\epsilon}\right|\right) \tag{13}$$

$$\Lambda_{1,2} = \frac{1}{t_f}\ln\left(\left|\frac{T_R\left(t_f, T_{R,0}\right) - T_R\left(t_f, T_{R,0}+\epsilon\right)}{\epsilon}\right|\right) \tag{14}$$

$$\Lambda_{1,3} = \frac{1}{t_f}\ln\left(\left|\frac{T_C\left(t_f, T_{C,0}\right) - T_C\left(t_f, T_{C,0}+\epsilon\right)}{\epsilon}\right|\right) \tag{15}$$

The deviation of each variable is calculated at a final time of $t_f = 500$ s, with an initial perturbation of $\epsilon = 10^{-3}$. Values for ϵ in the range of $10^{-1} - 10^{-4}\%$ of the variable analysed gave a good compromise between accuracy and numerical stability. If ϵ was made smaller, the deviation inside the logarithm can get close to zero, therefore resulting in large negative numbers. The control variable is given by the governing equation (16) for PI-controlled systems, and by 95% cooling for MPC controlled systems.

4. CONTROL SCHEMES

4.1 PI Control structure

The batch reactor temperature is controlled by varying the cooling water flow rate q_C with a PI controller. The equation of the used PI controller is given by:

$$u\left(t\right) = K_p\,\left(T_R\left(t\right) - T_{sp}\left(t\right)\right) + \frac{1}{\tau_I}\int_{t_0}^{t}\left(T_R\left(t'\right) - T_{sp}\left(t'\right)\right)dt' \tag{16}$$

where K_p is the proportional parameter, τ_I is the integral parameter, $T_{sp}\left(t\right)$ is the set point temperature at time t, $u\left(t\right)$ is the control value and t' is a dummy variable. The parameters of the PI controller are given in Table 2. The PI controller regulates the coolant flow, therefore controlling the reactor temperature.

Table 2. Parameters for PI controller used in case studies.

Parameter	Value
Proportional (P), K_p	10 $\mathrm{m^3\,s^{-1}\,K^{-1}}$
Integral (I), τ_I	1000 $\mathrm{K\,s^2\,m^{-3}}$

The current PI control is solely used to show how a stable system can become unstable due to a thermal runaway. The resulting system can be used to judge how well the Lyapunov exponents predict the system stability. No attempt was made to tune perfectly the PI controller since this is not the purpose of the following case study.

4.2 Model Predictive Control structure

The analysis of stability for batch processes is incorporated into the classical MPC structure as shown in Figure 3.

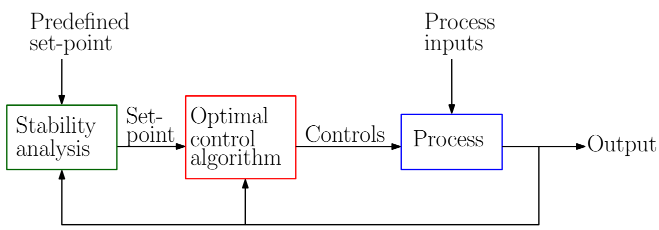

Fig. 3. Model Predictive Control scheme with integrated stability analysis.

Model Predictive Control (MPC) is an advanced control scheme, in which an Optimal Control Problem is solved iteratively (Chuong La et al., 2017). The mathematical formulation for MPC used in this work (Charitopoulos and Dua, 2016; Rawlings and Mayne, 2015) is given by:

$$\min_{u(\cdot)} \Phi\left(x\left(t\right), u\left(t\right)\right) \tag{17}$$

subject to the system described in (2) – (8) and:

$$\Phi = \int_{t_0}^{t_f} \left(T_R\left(t\right) - T_{sp}\left(t\right)\right)^2 dt \tag{18}$$

$$\Lambda_{l,i}\left(t_f\right) \leq 0 \qquad i = 1, 2, 3 \tag{19}$$

$$T_R \leq T_{chem} \tag{20}$$

$$0 \leq q_C \leq q_{C,max} \tag{21}$$

$$t_0 \leq t \leq t_f \tag{22}$$

where t_0 and t_f are the initial time and final time of the simulation, and the chemical stability temperature is set to $T_{chem} = 445$ K. In the above problem formulation the coolant flow rate q_C is equal to the control variable $u\left(t\right)$, *i.e.* $q_C = u\left(t\right)$. The constraint in (19) ensures that the process does not enter an unstable region at the end of the horizon considered, *i.e.* at $t = t_f$. This structure is different from that found in literature (Christofides et al., 2011), where Lyapunov functions are used.

The problem given in (17) - (22) is solved using the SQP optimisation (Nocedal and Wright, 2006) algorithm within *fmincon* in MATLAB™.

The algorithm proceeds with a "moving horizon": At time t the optimal control action is evaluated for a control and prediction horizon of $t_{control}$ and $t_{prediction}$, respectively. This scheme is shown diagrammatically in Figure 4.

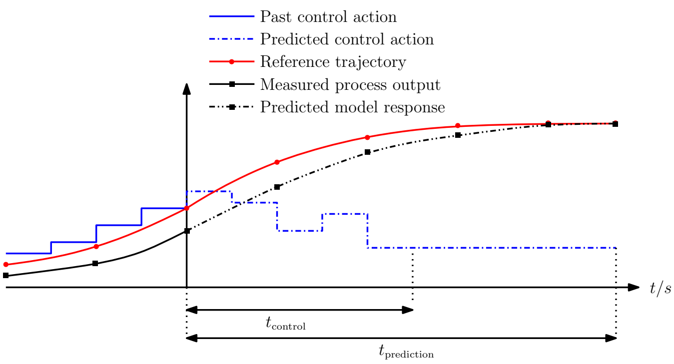

Fig. 4. Diagram of Model Predictive Control with control and prediction horizons t_{control} and $t_{\text{prediction}}$.

The control action found by the optimisation algorithm is implemented only for the first step. After every iteration the algorithm is fed with new process data which, together with the included process model, lead to new predictions of the system behaviour. With this information the optimisation is carried out to find the optimal control values.

5. CASE STUDIES OF BATCH REACTIONS

5.1 PI Control

An initially stable system is controlled using the PI control for the cooling jacket. At $t = 150$ s a step increase in the set point temperature of the reactor is implemented. This increase in the reactor temperature leads to an uncontrolled rise in temperature, which accelerates the rate of reaction. Since an exothermic reaction is present, this leads to a thermal runaway. The temperature profile of this process is shown in Figure 5.

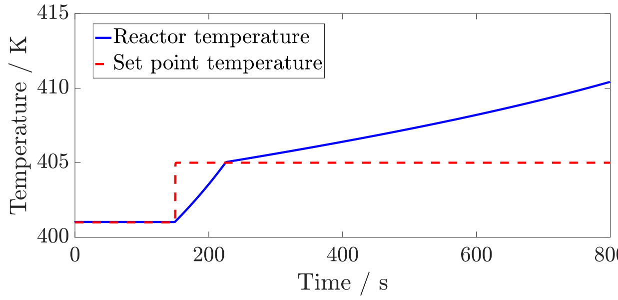

Fig. 5. Temperature profile of an exothermic batch reactor system. A step change in the set point temperature at $t = 150$ s leads to an unstable process.

It can be seen clearly from Figure 5 that at time $t \geq 200$ s the process turns unstable. A reliable stability criterion is required to identify this point of instability.

For each 10 s interval the Lyapunov exponent values are evaluated. For a time frame of 500 s this gives 50 evaluations per simulation. The reliability to detect instability, as well as the computational time required to calculate each respective criterion are tested.

The profiles for each Lyapunov exponent for the temperature profile given in Figure 5 are shown in Figure 6.

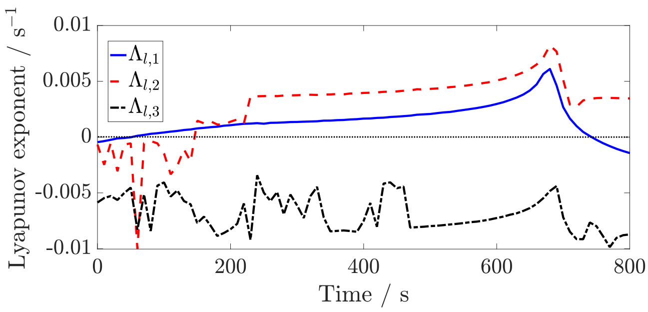

Fig. 6. Lyapunov exponent profiles for a batch process going out of control.

As can be seen in Figure 6 only the Lyapunov exponents predict the instability correctly. Before the new set point of 405 K is reached instability of the process is predicted. This instability is predicted at approximately 100 s. Therefore, the Lyapunov exponents are a reliable way of predicting instability of the batch process considered.

One issue with Lyapunov exponents is the computational cost: per iteration the system model has to be simulated with initial perturbations in order to quantify stability. As the problem size increases, this can become an issue for online control applications. For this system, which evaluates the stability for three state variables, approximately 140 ms were required per iteration.

5.2 Model Predictive Control

Process intensification, which can be achieved by using a stability constraint with MPC, is demonstrated in this section. As a comparison a process controlled by MPC with Lyapunov exponents and MPC with a constant set point temperature are shown. The target conversion of the batch process is set to 85%. The maximum temperature allowed is set to $T_{chem} = 445$ K, which is the chemical stability of the process. The temperature profiles for each process are shown in Figure 7.

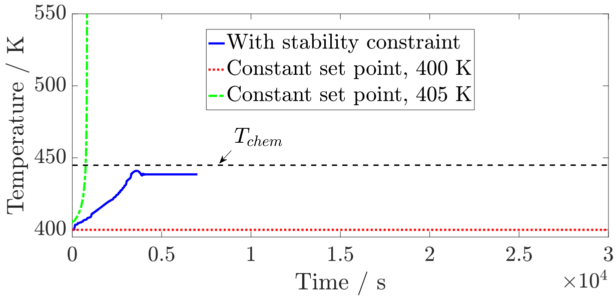

Fig. 7. Temperature profiles of batch processes controlled with MPC. For the process with constant set point of 405 K the temeprature increases beyond 550 K due to a thermal runaway.

The conversion profiles for each process are shown in Figure 8.

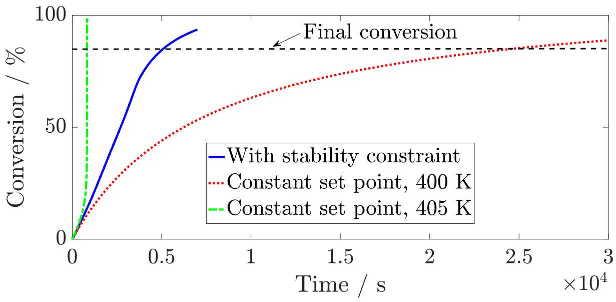

Fig. 8. Conversion profiles of batch processes controlled with MPC.

From Figure 8 it can be seen that the process including Lyapunov exponents as a stability constraint reaches the target conversion of 85% after 5,000 s in a controlled manner. The process with a constant temperature of 400 K needs 25,000 s. An increase of 5 K of the initial temperature already leads to an uncontrollable process. Therefore a significant decrease in reaction time (five-fold), whilst maintaining stability, was achieved with the inclusion of Lyapunov exponents as a measure of stability. This reduction of processing time results in earlier release of process units to be used for carrying out other tasks.

On average, each iteration for the MPC scheme with Lyapunov exponents required 1.48 s. A control horizon of $t_{\text{control}} = 20$ s was used for both processes. The complete nonlinear process model was used for the control scheme, as the linearisation of this system can potentially lead to wrong predictions of the system behaviour.

To further illustrate the advantages of using Lyapunov exponents implemented with MPC, two different MPC strategies are presented below:

- MPC with Lyapunov exponents, prediction horizon of $t_{\text{control}} = 20$ s, 1 step prediction
- MPC without stability constraints, prediction horizon of $t_{\text{control}} = 160$ s, 8 step prediction with 20 s per step

The performance for computational cost and stability are tested for the same batch reactor system, subject to an increase in set point temperature. The temperature profiles are shown in Figure 9.

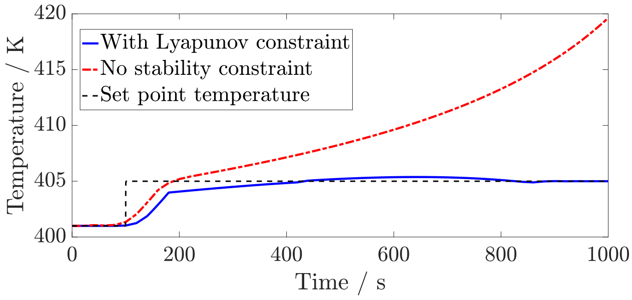

Fig. 9. Temperature profiles of batch processes controlled by Model Predictive Control with and without Lyapunov exponent constraints.

It can be seen from Figure 9 that the temperature profile for the MPC structure without stability constraints, but a larger control horizon, does not achieve the new set point temperature of 405 K in a stable manner. The resulting control profiles for the processes are shown in Figure 10.

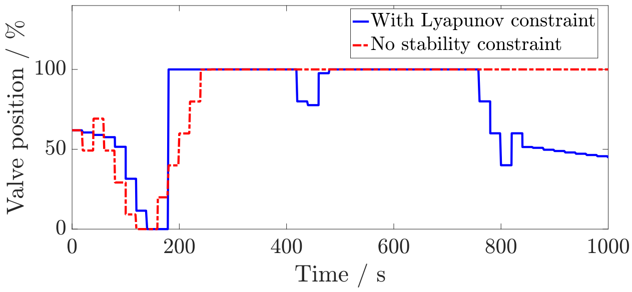

Fig. 10. Temperature profiles of batch processes controlled with MPC.

In Figure 10 it can be seen that the coolant flow for the process controlled by MPC with Lyapunov exponents increases rapidly just before $t = 200$ s as the boundary of instability has been reached.

The Model Predictive Control structure including Lyapunov exponents as a constraint achieves a stable process, even though the control horizon is only $1/8^{\text{th}}$ of the standard MPC formulation.

The average computational cost for each MPC structure without the use of stability constraints and a control horizon of $t_{\text{control}} = 160$ s was 2.3 CPU seconds, whereas the MPC implementation using Lyapunov exponent constraints and a control horizon of $t_{\text{control}} = 20$ s required an average of 2.0 CPU seconds. An MPC scheme with a control horizon of 500 s could be used, but with a larger horizon and more control intervals the optimisation problem increases, as well as the computational cost.

Hence, the MPC structure using Lyapunov exponents as stability constraints not only improves the stability of the system, but also reduces the prediction horizon necessary and hence the computational cost of the optimisation algorithm. These are clear advantages to standard MPC strategies. This can lead to improved safety of operation for systems controlled by MPC in industry, which reduces financial loss due to interruptions of normal operation.

Problems still arise when using Lyapunov exponents as a stability criterion for nonlinear systems. The horizon over which the Lyapunov exponents are evaluated needs tuning, leading to varying results depending on the system. For exothermic batch reactions considered in this work Lyapunov exponents predicted the system stability reliably.

6. CONCLUSIONS AND FURTHER WORK

A short review of common stability criteria for dynamic systems was presented. Key features of the Routh-Hurwitz criterion, Lyapunov exponents and the divergence criterion were given. The underlying theory of Lyapunov exponents was introduced and derived for the exothermic batch reactor system analysed. Additionally, the control systems used were explained and the implementation of Lyapunov exponents with Model Predictive Control (MPC), which is a novel control structure, was outlined.

Advantages of using Lyapunov exponents as a measure of stability are the simple implementation and the reliability of the results obtained, once tuned correctly.

Disadvantages include the need to tune the simulation horizon for Lyapunov exponents, as well as the computational cost as the problem size increases.

From the MPC case studies it was shown that for unstable systems of small size, the MPC implementation using Lyapunov exponents resulted in a computationally cheaper and more stable process than the standard MPC implementation using a larger control horizon. More case studies of larger systems are required to prove this property.

Furthermore, the use of Lyapunov exponents for a highly nonlinear system needs to be tested individually: there is no guarantee that Lyapunov exponents will give a correct prediction of system stability for every process. For batch reaction systems considered in this work Lyapunov exponents gave very reliable results.

The use of Lyapunov exponents with MPC for an exothermic batch reaction lead to a profound decrease in reaction time. This is due to the capability of predicting the system stability along the process trajectory. Hence an intensification of the process was enabled while keeping the process under control at all times.

This work has presented a totally new way of stabilising thermal runaway systems with an online MPC algorithm, while enhancing safety and performance of processes that can become unstable with detrimental effects leading to economic loss. The case studies presented demonstrate the benefits over traditional control approaches, as well as the enhanced ability to intensify the underlying processes so as to achieve greater productivity. The implementation of such MPC schemes requires the direct use of highly nonlinear mechanistic process models for dynamic, *i.e.* non steady-state, systems because linearisation is not representative for fast dynamic regions. Hence many control steps are necessary for equivalent standard MPC schemes.

Future work will continue by considering other, more complex reaction systems, as well as the impact of parametric uncertainty in the underlying process models used within the MPC scheme.

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