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Nonlinear Model Predictive Control of Dimethyl Ether Combustion in a Jet Stirred Reactor ⋆

Thomas Lammersen * **Klaus-Dieter Stoehr** **
Norbert Peters *** **Dirk Abel** ****

* *Institute of Automatic Control, RWTH Aachen University, Aachen. e-mail: t.lammersen@irt.rwth-aachen.de*
** *Institute for Combustion Technology, RWTH Aachen University, Aachen. e-mail: k.d.stoehr@itv.rwth-aachen.de*
*** *Institute for Combustion Technology, RWTH Aachen University, Aachen. e-mail: n.peters@itv.rwth-aachen.de*
**** *Institute of Automatic Control, RWTH Aachen University, Aachen. e-mail: d.abel@irt.rwth-aachen.de*

Abstract: This work focuses on the nonlinear control of instabilities in the combustion of a diluted dimethyl ether (DME) / air mixture under low temperature conditions. A nonlinear model predictive control (NMPC) is utilized to stabilize the combustion in simulation with the aim to specify minimum actuation dynamic requirements and develop control strategies for an existing experimental chemical reactor.

1. INTRODUCTION

Common experimental setups for gathering reaction and kinetic data of combustion processes are based upon shock tubes, flow- or stirred reactors in which the reaction takes place. This work focuses on a continuous jet stirred reactor (CSTR) operated by the CRC 686 at low-temperature conditions. Under these conditions the reactor system is showing an oscillatory behavior resulting from periodical ignitions and quenching effects. Because of the importance of low-temperature combustion for emission reduction, the dynamics of low-temperature oscillations and damping by active control methods is a subject of research in the CRC.

In preliminary works Jarmolowitz et al. [2009] applied a MPC using a trajectory piecewise linear model (TPWL) to control the reactor system and gain a steady and continuous combustion process for the operation with a methane-air mixture. A further approach used a one-step reaction model to control oscillations occurring during the combustion of methane, see Wada et al. [2011]. Due to the more complex ignition process of dimethyl ether (DME) a one-step model is not able to capture the dynamics of this process in a sufficient way. Lammersen et al. [2013] applied a linear model predictive control using a detailed chemical reaction mechanism by Beeckmann et al. [2010]. Because of the extreme dynamics of the reactor, the resulting system of differential equations shows eigenvalues with large magnitudes and both signs. Although the linear MPC is capable of stabilizing the system in simulations, there are two major drawbacks: First, the resulting control trajectory would require a very high actuation dynamic. Second, and even more important is, that a stabilization with a linear MPC was only possible by using a nonlinear prediction of the free system response. Due to the systems unstable behavior and the numerical properties a single-shooting forward simulation is not possible for relevant horizon lengths under real-time conditions, therefore not applicable to the experimental setup.

This work is evaluating the use of a nonlinear model predictive control to stabilize the reactor system using the multiple-shooting principle introduced by Bock and Plitt [1983]. The control results are then used to specify minimum requirements to the actuation system while the possibility of parallel evaluation of the horizon prediction can be used to establish real-time capability on a multi-core HIL-system which is available to the CRC 686. The reactor temperature as well as the concentrations of all species occurring during the combustion process are reconstructed by an extended Kalman filter using a cumulated carbon hydrogen (CH) concentration signal and a temperature signal provided by a flame ionization detector. The controller setup is using the equivalence ratio ϕ defined as

$$\phi = \frac{3 \cdot X_{DME}}{X_{O2}} \quad , \tag{1}$$

with the inlet mole fractions of dimethyl ether (X_{DME}) and oxygen (X_{O2}) and the residence time of the gas mixture inside the reactor τ as manipulated variables. A mixture with $\phi = 1$ is a stoichiometric fuel / oxygen mixture. After a short description and a brief overview of the modeling approach for the reactor system, the used observer and MPC are presented, followed by a discussion of the results.

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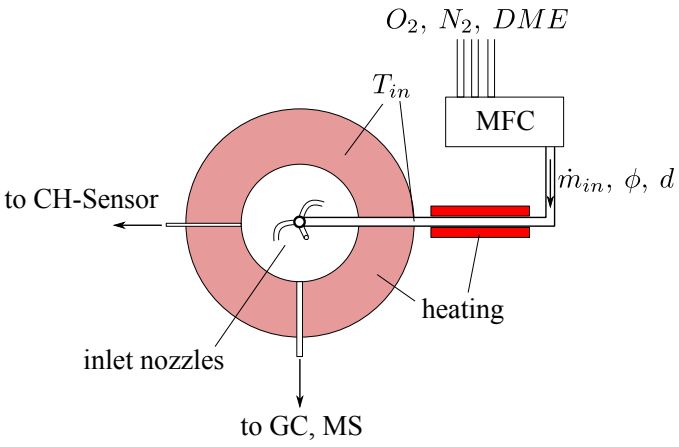

Fig. 1. Sketch of the experimental setup

2. JET STIRRED REACTOR

2.1 Experimental setup

Fig. 1 shows a sketch of the experimental setup. The JSR itself consists of a glass bulb with three fuel nozzles, ensuring a homogeneous mixture inside the reactor. The fuel nozzles are fed by a preheated fuel, oxygen and nitrogen mixture from the mass flow controllers (MFC). The burned mixture is exiting the reactor through the exhaust line leading to gas chromatography and mass spectrometry systems, while a small amount of burned gas is sucked into the inlet of the CH-FID-sensor. To minimize heat losses through the wall and ensure a well defined boundary condition for simulation purposes, the complete JSR is surrounded by a heating and an insulation which keeps the relevant ambient temperature at inlet temperature T_{in}.

The operating conditions are given by the composition, temperature and amount of the inlet gas stream, defined by the actual gas mixture, the equivalence ratio ϕ, the dilution with nitrogen d, the temperature T_{in} and the massflow $\dot{m}_{in}$ of the mixture. Since the reactor is working as a continuous system, the mass of gas inside the reactor will assumed to be constant, resulting in $\dot{m}_{in} = \dot{m}_{out}$. According to usual practice, the inlet massflow will be substituted by the residence time

$$\tau = \frac{\rho V}{\dot{m}_{in}}$$

where V denotes the reactor volume and ρ the density of the inlet mixture. The main manipulated variable for stabilization purposes in this work is the equivalence ration ϕ

The signal produced by the CH-sensor corresponds to the cumulated concentrations of several species with different weighting coefficients. These coefficients are available for a broad spectrum of species in literature. In this work the weighting factors supplied by Dietz [1967] are used.

2.2 Modeling of the Jet Stirred Reactor

The reactor model is based upon a chemical reaction mechanism published by Beeckmann et al. [2010] describes the oxidation of dimethyl ether by a 49-step reaction scheme involving a total of 31 different chemical species including several radicals which are occurring during the combustion process. Therefor the reactor can be modeled as an open thermodynamical system with one energy conservation equation and a mass balancing equation per each species, resulting in a system of 32 differential equations.

The balancing equations are

$$c_p\,\rho\,V\frac{dT}{dt} = (\Delta h_{in} - \Delta h_{out})\cdot\dot{m}_{in} - \dot{Q}_{loss} + \dot{Q}_{chem} \quad (2)$$

and

$$\rho\,V\,\frac{dY_j}{dt} = (Y_{j,in} - Y_j)\cdot\dot{m}_{in} + \dot{m}_{j,chem} \quad (3)$$

for $1 \le j \le N_S$. c_p, V, ρ, α, A, T_{amb} are specific heat capacity, reactor volume, density, wall heat transfer coefficient, reactor surface area and ambient temperature, N_S is denoting the number of species. Δh_{in} is the specific enthalpy of the inlet mixture, Δh_{out} is the specific enthalpy of the current reactor mixture relative to the reference enthalpy at normal conditions ($T_0 = 300K$).

The heat loss through the reactor wall evaluates to

$$\dot{Q}_{loss} = \alpha\,A\,(T - T_{amb}) \quad , \quad (4)$$

while the chemical source terms are given by

$$\dot{Q}_{chem} = -V\cdot\sum_{j=1}^{N_S} v_j\cdot h_{j,m} \quad (5)$$

and

$$\dot{m}_{j,chem} = V\cdot M_j\cdot v_j\,, \quad (6)$$

where N_S is the total number of species and v_j, $h_{j,m}$ and M_i denoting the net production rate, the molar enthalpy and the molar weight of species j. The thermodynamical properties ($c_{p,j,m}$, $h_{j,m}$) are calculated by making use of the NASA polynomials, while the chemical production rates are calculated as described in Lammersen et al. [2013]. Detailed information on the used modeling approach can be found in Poinsot and Veynante [2005]. The model can then be written in standard state space form

$$\dot{x} = f\,(x,u) \quad (7)$$

with

$$f\,(x,u) = \begin{pmatrix} \dfrac{dT}{dt} \\ \\ \dfrac{dY_j}{dt} \end{pmatrix}, \quad i = j..N_S \quad , \quad (8)$$

and the state vector x and input vector u, given by

$$x = \begin{pmatrix} T \\ Y_1 \\ \vdots \\ Y_{N_S} \end{pmatrix} \text{ and } u = \begin{pmatrix} T_{in} \\ \tau \\ d \\ \phi \end{pmatrix}. \quad (9)$$

3. CONTROL SYSTEM

3.1 State observer

Since the current experimental setup is only supplying temperature and a HC concentration as measurement data, the full system state required by the MPC is being reconstructed by an extended Kalman filter, i.e. a non-linear prediction is corrected by using a linear updated covariance matrix:

$$\mathbf{P}_{k|k-1} = \mathbf{A_{k-1}}\mathbf{P}_{k-1}\mathbf{A_{k-1}} + \mathbf{Q_{k-1}}\,, \tag{10}$$

where $\mathbf{P}$, $\mathbf{Q}$ and $\mathbf{A}$ are denoting the covariance matrix, state noise covariance matrix and the linear state transition or sensitivity matrix. Due to the very limited sensor information available an exact determination of the state transition matrix is crucial for state vector reconstruction. Due to performance requirements of an exact sensitivity calculation using

$$\frac{\partial \mathbf{A_{k-1}}}{\partial t} = \frac{\partial}{\partial x} f(x,u) \tag{11}$$

is not applicable. The exact linear solution

$$\mathbf{A}_{k-1} = \exp\left(\tilde{\mathbf{A}}\Delta t\right) \tag{12}$$

with $\tilde{A} = \frac{\partial f}{\partial x}$ is especially for large matrices with large norms (see Higham [2005]) very expensive and thus unsuitable for real-time application in this case. Instead the approximation

$$\mathbf{A}_{k-1} = \left(\mathbf{I} + \frac{\Delta t}{2}\tilde{\mathbf{A}}\right)^{-1}\left(\mathbf{I} - \frac{\Delta t}{2}\tilde{\mathbf{A}}\right) \tag{13}$$

with the identity matrix $\mathbf{I}$ is used. This approach is still more expensive than the simple approach $\mathbf{A}_{k-1} = \mathbf{I} + t\tilde{\mathbf{A}}$ but accounting for model stiffness and avoiding numerical instabilities because of its implicit character. Fig. 2 shows a comparison between simulation and experimental results. The simulated model is showing an offset in temperature and DME concentration. The exact reason for this offset is subject of current work and not yet fully explainable. As the closeup in the lower two graphics shows that the simulation is exactly matching the oscillation frequency and phase. A further model validation would require more measurement signals which are not available at the current point. In this work it is therefor assumed that the model is reflecting the system behavior in a sufficient way.

3.2 Multiple Shooting NMPC

To stabilize the reactor system, a nonlinear MPC is being used in this work. The overall task is to solve the problem

$$\min_{u(\cdot)} J(u(\cdot), x(\cdot)) \tag{14}$$

$$s.t.\ \dot{x}(t) = f\left(x\left(t\right)\right), u\left(t\right))) \tag{15}$$

$$\mathbf{C}_x\, x(\cdot) \leq b_x \tag{16}$$

$$\mathbf{C}_u\, u(\cdot) \leq b_u \tag{17}$$

where the convex cost function is defined as

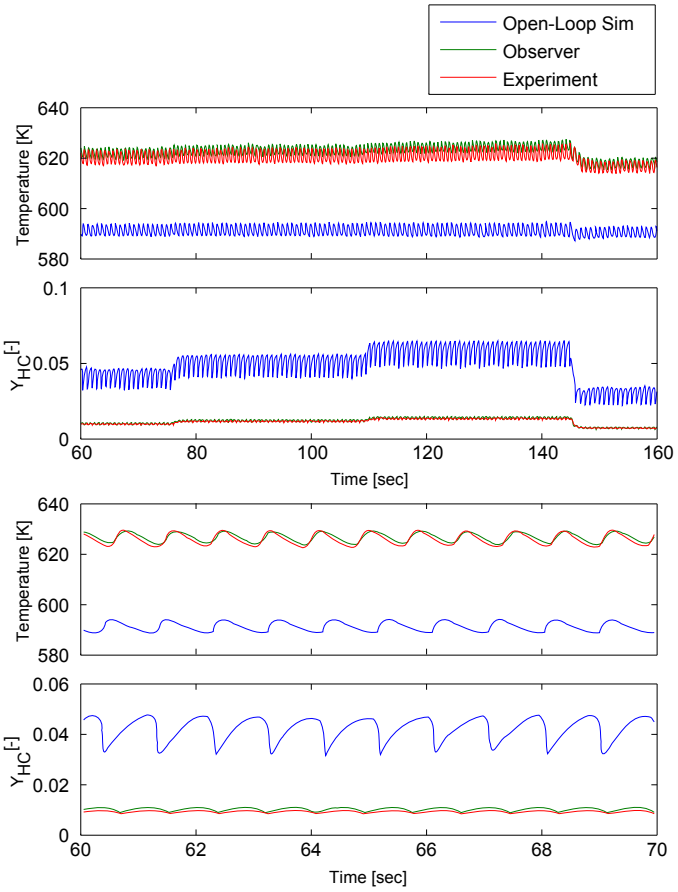

Fig. 2. Comparison of simulation, experiment and observer results for Temperature and DME mass fraction in two different time resolutions

$$J(u(\cdot), x(\cdot)) = \sum_{i=1}^{H_2} \left(x(t_i) - x_{ref}\right)^T \mathbf{Q}_i \left(x(t_i) - x_{ref}\right) + \sum_{j=0}^{H_u - 1} \left(u(t_j) - u_{ref}\right)^T \mathbf{R}_j \left(u(t_j) - u_{ref}\right)^T \tag{18}$$

As in most MPC applications, the system state at a given time t_k is defined by an initial system state $x(t_0)$ and the past inputs $u(t_0), ..., u(t_k)$. Applying a multiple shooting algorithm, this connection can be resolved by an iterative procedure of forward simulation and solution of sequential quadratic by programs Bock and Plitt [1983].

Let $x_{n,k}$ be an approximation to $x(t_k)$ and $u_{n,k} \approx u(t_k)$. Using an arbitrary discretization scheme the differential equality constraint (15) can be turned into the discrete equation

$$x_{n,k+1} = F(x_{n,k}, u_{n,k}) \quad . \tag{19}$$

Using a past solution (index $n-1$) (19) can be linearized, resulting in the recursion

$$x_{n,1} = x_{n-1,1} + \mathbf{S}_{u,k}\left(u_{n,k} - u_{n-1,k}\right) \tag{20}$$

$$x_{n,k+1} = x_{n-1,k+1} + \mathbf{S}_{x,k}\left(x_{n,k} - x_{n,k-1|k}\right) + \mathbf{S}_{u,k}\left(u_{n,k} - u_{n-1,k}\right) \tag{21}$$

with the sensitivity matrices

$$\mathbf{S}_{x,k} = \frac{\partial F(x_{n,k-1}, u_{n,k})}{\partial x_{n,k-1}} \text{ and } \mathbf{S}_{u,k} = \frac{\partial F(x_{n,k-1}, u_{n,k})}{\partial u_{n,k-1}} \quad (22)$$

and the one step prediction

$$x_{n,k-1|k} = F(x_{n-1,k-1}, u_{n-1,k-1}) \quad . \quad (23)$$

Using the block matrices

$$\mathbf{V}_x = \begin{pmatrix} \mathbf{0} & & & \\ \mathbf{S}_{x,1} & \mathbf{0} & & \\ & \mathbf{S}_{x,2} & \mathbf{0} & \\ & & \ddots & \ddots \end{pmatrix} \quad (24)$$

and

$$\mathbf{V}_u = \begin{pmatrix} \mathbf{S}_{u,1} & & \\ & \mathbf{S}_{u,2} & \\ & & \ddots \end{pmatrix} \quad (25)$$

the differential constraint (15) is finally turned into a algebraic equality constraint

$$(\mathbf{I} - \mathbf{V}_x \quad -\mathbf{V}_u) \cdot \begin{pmatrix} X_{n+1} \\ U_{n+1} \end{pmatrix} = X_n - \mathbf{V}_x \tilde{X}_n - \mathbf{V}_x U_{n-1} \quad (26)$$

using

$$X_n = \begin{pmatrix} x_{n,1} \\ \vdots \\ x_{n,H_2} \end{pmatrix} \quad U_n = \begin{pmatrix} u_{n,0} \\ \vdots \\ u_{n,H_u-1} \end{pmatrix} \quad (27)$$

and

$$\tilde{X}_n = \begin{pmatrix} x_{n,0|1} \\ \vdots \\ x_{n,H_2-1|H_2} \end{pmatrix} \quad (28)$$

Starting now from an initial solution X_0 and U_0 the prediction vector $\tilde{X}_1$ can be calculated by evaluating H_2 one step forward predictions (23) using the current input vector U_0. Since these prediction steps are not relying on each other they can a) be evaluated in parallel and b) an unstable system behaviour is only carried further for one prediction step.

Solving (14) with constraints (15) through (17) and (26) with an arbitrary QP-Solver gives an updated solution X_n and U_n. Iterating this process then leads to a solution of the nonlinear optimal control problem.

3.3 Implementational remarks

Discretization A consequence of the harsh numerical properties of the model equations is, that discretization using a fixed time step approximation requires unrealistic small time step sizes. Here a variable-step BDF-solver (see Hairer and Wanner [2010]) was used, yielding acceptable average time step sizes.

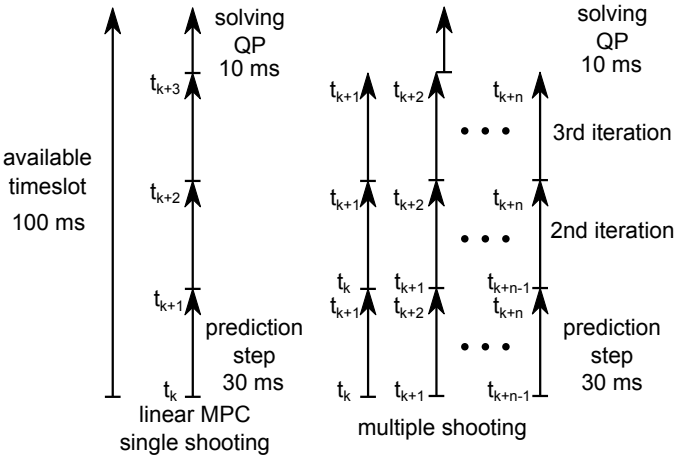

Fig. 3. Comparison between single shooting or linear MPC with the multiple shooting approach.

Calculation of the sensitivity matrices: Since (19) is only implicitly defined by applying the BDF-solver to (7) the sensitivity matrices $\mathbf{S}_{x,k}$ and $\mathbf{S}_{u,k}$ cannot be evaluated analytically but are themselves solutions of the ODEs

$$\dot{\mathbf{S}}_x = \frac{\partial}{\partial x}\dot{x} = \left(\frac{\partial f}{\partial x}\right)^T f(x,t) \quad (29)$$

$$\dot{\mathbf{S}}_u = \frac{\partial}{\partial u}\dot{x} = \left(\frac{\partial f}{\partial u}\right)^T f(x,t) \quad . \quad (30)$$

An exact solution would result in an extreme computational effort, instead a linear approximation to the state transition matrix

$$S_x = \exp\left(\tilde{\mathbf{A}}\Delta t\right) \quad (31)$$

is used, where again $\tilde{A} = \frac{\partial f}{\partial x}$. This matrix is than evaluated by the approximation (13) used in the EKF as well.

Condensation and Solution The disadvantage of the multiple shooting approach is, that the model equations are explicitly treated as constraints resulting in a large number of additional constraints compared to a linear MPC approach. Here a condensation technique introduced by Bock and Plitt [1983] and described by Peifer and Timmer [2007] in detail was applied to reduce the resulting QP-problem to the same size a linear MPC would require. The resulting QP-Problem is solved by using qpOASES Ferreau et al. [2008].

Parallelization At the current point the nonlinear forward simulation of the reactor system can be performed in about 30% of real time, i.e. to calculate $100ms$ of system behavior $30ms$ are needed. It follows, that for any form of nonlinear prediction further than three steps ahead a sequential calculation is not possible (see fig. 3). Since even the linear MPC requires a nonlinear prediction of the free control variable due to the numerical properties of the reactor system, neither a linear nor a single shooting approach are estimated to work on the experimental setup.

MPC setup		**Inlet conditions**	
pred. horizon length	10	dilution with nitrogen	80%
control horizon length	10	residence time	$0.5s$
sampling time	0.01 s	fuel equivalence ratio	0.85
controlled variable	T		
manipulated variable	ϕ		

Constraints and Penalties

state constraints	-
ϕ (absolute)	$0.2 \leq \phi \leq 2$
$\Delta\phi$	$-0.1 \leq \Delta\phi \leq 0.1$
state penalty Q_i	0.001
input penalty R_i	1

Table 1. Data for simulations

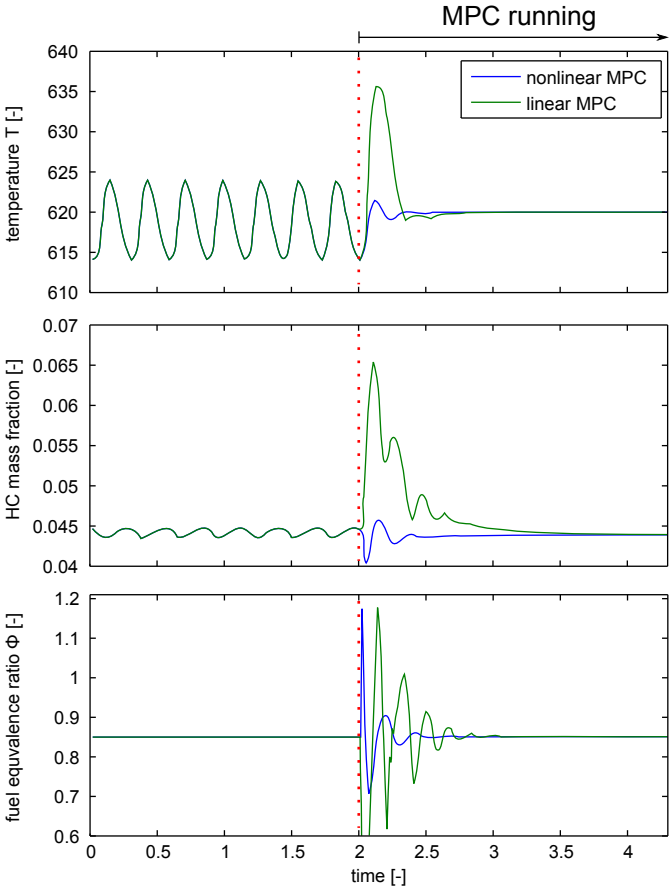

Fig. 4. Comparison of simulation results with linear and nonlinear MPC for reactor temperature (top), HC mass fraction (middle) and input trajectory (bottom)

4. CONTROL RESULTS

The multiple shooting MPC was applied to a simulation of the reactor to gain experience regarding the system behavior and dynamics as well as to get a theoretical minimum of necessary actuation dynamics to control and stabilize the combustion process in the experimental setup. In the simulation the parameter shown in table 4 have been used.

As the controlled variable the reactor temperature is used. The manipulated variable is the fuel equivalence ratio ϕ.

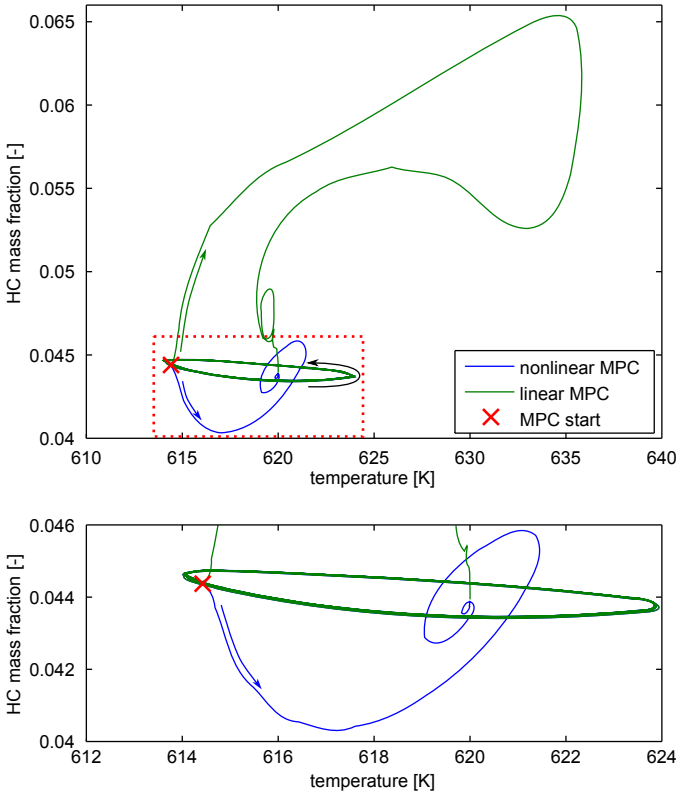

Fig. 5. Phase diagram of temperature / HC mass fraction curve of the reactor system with linear MPC and nonlinear MPC (top) and a closeup to the marked area (bottom).

Figure 4 shows the results of the control simulation. Without the MPC running, the reactor temperature is oscillating in a stable limit cycle. At $t = 2s$ the controller is turned on and damping out the oscillations. The comparison between the linear MPC presented in Lammersen et al. [2013] and the now implemented nonlinear multiple shooting NMPC demonstrates the structural advantages of the NMPC scheme. The temperature and HC results in the top and middle figure are showing a significant overshooting for the system controlled with the linear MPC. The resulting input trajectories are plotted in the bottom figure. Although the control actions are less aggressive, the total duration of the damping phase is about half a second shorter when using an NMPC and the generated control trajectory is easier to be reproduced on the experimental setup by the mass flow controllers.

A phase plot of the reactor state trajectory in the temperature / HC - space is shown in fig. 5. The arrows are marking the traversing directions. Clearly visible is the systems limit cycle without active control forming the elliptic trajectory in the red rectangle. When the controller is switched on the system is leaving the limit cycle temporarily before running into its stable point within the limit cycle. The system behavior is confined to a much smaller area when controlled by a nonlinear MPC compared to the result when applying a linear MPC.

The tracking behavior of the controlled system for a variable reference is shown in fig. 6. The controller is turned on at $t = 1s$. Again, the linear MPC leads to

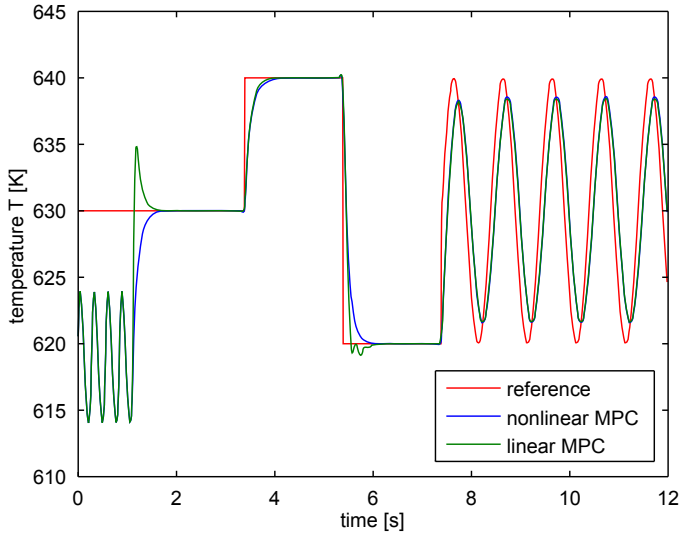

Fig. 6. Transient system behavior on variable referenc.

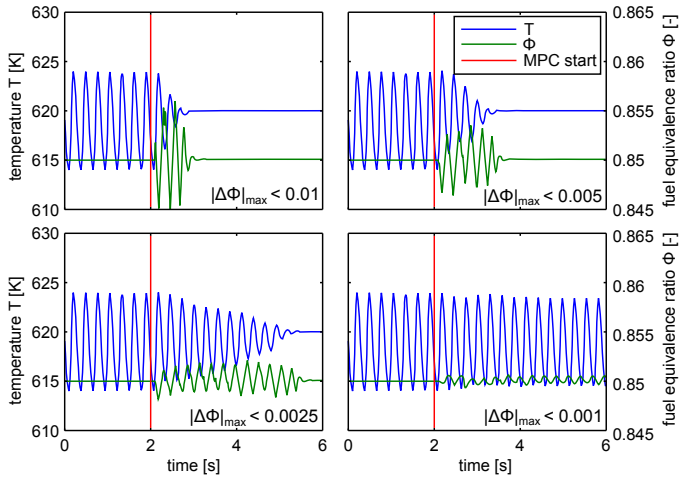

Fig. 7. Control results with limited actuator dynamics

significant overshooting amplitudes when sudden changes are applied to the reference. For smooth changes in the reference a difference in the performance of the linear and nonlinear controller is not detectable.

A possible approach to identify minimum actuation dynamics is to tighten the constraints for the maximal change in the manipulated variable up to the point where a stabilization is not possible anymore. Starting from $|\Delta\phi| < 0.01$ several simulations were performed to identify a critical constraint. The results are shown in fig. 7. A stabilization could not be achieved anymore, if $|\Delta\phi|$ is bounded to 0.001 while 0.0025 was still sufficient. Considering a total operating range of the inlet mass flow controllers of $0.2 \leq \phi \leq 2$ and the MPC sampling time of $\Delta t = 0.01$ a change of about 14% of the total range per second can therefor regarded es sufficient to control the experimental setup.

5. CONCLUSION

It was demonstrated that an oscillating chemical combustion system can be controlled and stabilized with a nonlinear model predictive control using a detailed chemical model, evaluated using a multiple shooting approach. The results have been compared to the results in a preliminary work where a linear MPC has been used. The nonlinear approach is showing a significantly better performance regarding actuation requirements and duration of the damping phase. As an important result minimum requirements of the mass flow controller performance in the experiment could be derived. The required actuation dynamics lies well within the capacity of commercially available products.

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