Model Predictive Control of Dimethyl Ether Combustion in a Jet Stirred Reactor under Low Temperature Conditions

Thomas Lammersen*, Klaus Stoehr†, Norbert Peters† and Dirk Abel*

*Institute of Automatic Control, RWTH Aachen University, 52074 Aachen, Germany
† Institute for Combustion Technology, RWTH Aachen University, 52074 Aachen, Germany

Email: {t.lammersen, d.abel}@irt.rwth-aachen.de, {K.Stoehr, N.Peters}@itv.rwth-aachen.de

Abstract—This paper deals with the control of instabilities and oscillations during the combustion of dimethyl ether (DME) in a continuous jet stirred reactor (JSR). A Model Predictive Control (MPC) is applied to keep the reactor in a steady state at low temperature combustion conditions. The full chemical state of the system consisting of temperature and species concentration is reconstructed from a temperature and a CH concentration signal by an extended Kalman filter. For prediction within the MPC and the filter, a physical model of the JSR including a full combustion reaction mechanism is presented.

I. INTRODUCTION

The Collaborative Research Center 686 (CRC686), funded by the German Research Association (DFG) is dedicated to the research in the control of low-temperature combustion processes. For the application of modern control techniques a well based system knowledge is of crucial importance, thus several subprojects deal with basic research in the field of combustion chemistry and reaction kinetics. Common experimental setups for gathering reaction and kinetic data of combustion processes are based upon shock tubes (eg. [4]) or flow reactors (eg. [5]) in which the reaction is taking place.

For combustion mechanism research, the CRC686 is operating a continuous Jet Stirred Reactor (JSR) at steady combustion condition to provide a constant flow of exhaust gases for analysis by mass spectrometry (MS) and gas chromatography (GC). Under several fuel-dependent combinations of inlet conditions, the gas mixture in the JSR is igniting and quenching periodically, spoiling the GC and MS measurements for further chemical analysis. Especially under low temperature conditions a steady combustion is not achieved. Due to the importance of low-temperature combustion for pollutant reduction, a stabilization of the reactor system and thus the possibility to get reliable GC and MS data would provide a good basis for future research.

For the operation with a methane-air mixture, Jarmolowitz applied a MPC based on a trajectory piecewise linear model (TPWL) derived by numerical differentiation [6]. An additional approach used a one-step reaction model derived by Wada [7] in combination with a non-linear MPC. This paper will examine the control of instabilities during the operation of the JSR with a diluted DME-air mixture. Although stability issues of this setup at certain points of operations are well known [10], a stabilization via closed loop control was not performed up to now.

Due to the much higher complexity of the combustion process of DME compared to the combustion of methane, a one-step model is not able to capture the reaction in a sufficient level of detail, so a more detailed reaction scheme has to be used. Combustion reaction systems show a very dynamical behavior including several different time scales, starting from less than a millisecond up to several seconds. This results in local eigenvalues in a wide range of magnitude with both, positive and negative sign, resulting in a stiff system of differential equations.

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 \( \phi \) and the residence time of the gas mixture inside the reactor \( \tau \) as manipulated variables.

II. JET STIRRED REACTOR

A. Experimental setup and definitions

Fig. 2 shows a sketch of the experimental setup. The JSR itself consists of a glass bulb with three fuel nozzles, arranged at an angle of 120 degrees in the center. The fuel nozzles are connected to the feed line which passes the preheating device and then connects to the mass flow controllers (MFC) which are delivering fuel, oxygen and
nitrogen at a defined rate. After combustion, the main share of the burned mixture leaves the JSR through the exhaust line leading to the GC and MS 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 $\phi$, the dilution with nitrogen $d$, the temperature $T_{in}$ and the massflow $m_{in}$ 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 $\rho$ the density of the inlet mixture.

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 factor supplied in [2] are used.

B. Experimental results

Wada and Peters[9] divided the range of operation point into five different regimes with respect to $T_{in}$ and the equivalence ratio $\phi$. Fig. 2 shows the resulting diagram, taken from [9]. If $T_{in}$ is too small, no ignition will occur (regime I). With increasing inlet temperature the reactor will enter the regime of low temperature combustion. Depending on the selected equivalence ratio $\phi$ the combustion process can enter an oscillating limit cycle (regime II), where sudden ignition and quenching occurs. Further increase of $T_{in}$ leads to a stable combustion (III) until the range of high temperature oscillations is reached (regime IV), a transient temperature plot of raw and filtered sensor data is shown in fig. 3. For even higher $T_{in}$ the process becomes stable again (V).

Due to the importance of low-temperature combustion in pollutant reduction and lowering formation of nitrous oxides (NOx) this paper is mainly dealing with oscillations under low-temperature conditions in regime II.

III. MODELLING OF THE JET STIRRED REACTOR

The model can be roughly divided into two components. The first part are the actual differential equations for the conservation of energy in the reactor and the conservation of the masses of each species. The second part is the chemical kinetics engine which calculates heat release and species production to resolve the corresponding chemical source terms in each iteration.

A. Differential equations

The reactor is modeled as an open thermodynamical system by one energy conservation equation and a mass conservation equation per occurring species. Assuming constant pressure and constant mass of gas inside the reactor (i.e. $\dot{m}_{in} = \dot{m}_{out}$) the balancing equations are

$$c_p \rho V \frac{dT}{dt} = (\Delta h_{in} - \Delta h_{out}) \cdot \dot{m}_{in} - \alpha A (T - T_{amb}) + \dot{Q}_{chem}$$

(1)

and

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

(2)

for $1 \leq j \leq N_S$, $c_p$, $V$, $\rho$, $\alpha$, $A$, $T_{amb}$ 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. $\Delta h_{in}$ is the specific enthalpy of the inlet mixture, $\Delta h_{out}$ specifies the specific enthalpy of the current reactor mixture relative to reference enthalpy at normal conditions ($T_0 = 300K$). As inlet mixture...
a diluted fuel-air mixture is used, so all species except for DME, O\textsubscript{2} and N\textsubscript{2} will have zero inlet mass fractions \(Y_{j,in}\).

The chemical source terms are given by

\[
\dot{Q}_{chem} = -V \cdot \sum_{j=1}^{N_S} v_j \cdot h_{j,m}
\]

and

\[
\dot{m}_{j,chem} = V \cdot M_j \cdot v_j,
\]

where \(N_S\) is the total number of species and \(v_j, h_{j,m}\) and \(M_j\) denoting the net production rate, the molar enthalpy and the molar weight of species \(j\). Since \(v_j\) and \(h_{j,m}\) are functions of the current state, they have to be calculated every iteration step.

The model can then be written as

\[
\dot{X} = f(X,U)
\]

with

\[
f(X,\Omega) = \begin{pmatrix} \frac{dT}{dt} \\ \frac{dY_j}{dt} \end{pmatrix}, \quad i = j..N_S,
\]

and the state vector \(X\) and input vector \(U\), given by

\[
X = \begin{pmatrix} T \\ Y_1 \\ \vdots \\ Y_{N_S} \end{pmatrix} \quad \text{and} \quad U = \begin{pmatrix} T_{in} \\ \tau \\ d \\ \phi \end{pmatrix}.
\]

**B. Calculation of chemical variables**

In this section the basic procedure for calculating production rates is provided for reference in later sections. Detailed description of the necessary calculations can be found in literature (e.g. [12]).

1) Thermodynamic properties: The thermodynamical properties \(c_{p,j,m}, h_{j,m}\) and the molar entropy \(s_{j,m}\) of the single species are computed by evaluating polynomials supplied by NASA at reactor as well as at inlet conditions. Since the species mass fractions \(Y_j\) are known, the corresponding model properties can easily be evaluated by

\[
f(T) = \sum_{j=1}^{N_S} \frac{Y_j}{M_j} \cdot f_{j,m}(T),
\]

substituting \(f(T)\) accordingly.

2) Rates of production: The production rates are calculated based on the used reaction scheme. For low temperature combustion, Beeckmann et al. reduced this scheme to a total of 49 equations, including 31 species [11], in the following referred to as 49S-Mechanism. Once the mechanism is known, the species’ production rates can be computed as follows.

For a standard reaction

\[
\nu_{i,A} S_A + \nu_{i,B} S_B = \nu_{i,C} S_C + \nu_{i,D} S_D
\]

with four species \(S_A, S_B, S_C\) and \(S_D\), the net rate of production \(\frac{dC_i}{dt}\) of species \(S_A\) by reaction \(i\) is given by

\[
\frac{dC_i}{dt} \bigg|_{i} = \nu_{i,A} \left(-k_{f,i} \cdot C_A^{\nu_{i,A}} \cdot C_B^{\nu_{i,B}} + k_{b,i} \cdot C_C^{\nu_{i,C}} \cdot C_D^{\nu_{i,D}} \right)
\]

whereas the rate coefficient \(k_f\) and \(k_b\) is determined by a standard Arrhenius approach of the form

\[
k_{f,i} = A_i \cdot T^{n_i} \cdot e^{-\frac{E_i}{T}},
\]

where the frequency factor \(A_i\), the preexponential factor \(n_i\) and the activation energy \(E_i\) are specified for each reaction in the used mechanism. The rate coefficient for the reverse reaction \(k_{b,i}\) can then be computed by

\[
\frac{k_{f,i}}{k_{b,i}} = K_{C,i},
\]

where the equilibrium coefficient \(K_{C,i}\) is a function mainly of species enthalpy, entropy and reaction order of reaction \(i\). If the rate coefficients are known, the net rates of production result in

\[
\frac{dC_i}{dt} = \sum_{i=1}^{N_{reactions}} \frac{dC_i}{dt} \bigg|_{i} = v_i.
\]

This approach works for most reactions, however some need a special treatment to account for additional pressure dependence and third body collisions, see [12] for details.

Especially (10) and (11) are leading to the highly nonlinear behavior of combustion systems. In the used mechanisms the frequency factor \(A\) is taking values in a range of \(10^9 \text{kmol}^{-1}\text{m}^{-3}\text{s}^{-1} \text{kmol}^{-3}\text{s}^{-1} \text{kmol}^{-3}\text{s}^{-1}\), resulting in a large spread in orders of magnitude for the corresponding rate coefficients.

**C. Validation**

The model was validated against offline measurements of the experimental setup obtained at \(T_{in} = 580K\), \(\tau = 0.35s\)
and $\phi = 0.5$. The frequency of temperature oscillations is met with little difference, however there is a not neglectable difference between simulated and observed oscillation amplitude.

The difference in amplitude is mainly caused by the dynamical behavior of the thermocouplers used to measure the gas mixture temperature. They are showing a first-order-lag behavior with a large time constant compared to the combustion time scale and are therefore not able to follow oscillations to the full extend. A second problem arises from the operating range of the used sensors. Since the thermocouplers are designed to be operated at temperatures up to 1500K they are showing large disturbances, which can be seen in figure 3.

The author assumes that the slight frequency mismatch is caused by the open system assumption. As mentioned before, the reactor is modeled as a thermodynamically open system. As a result the pressure inside the reactor is assumed to be constant and equal to ambient pressure. In the real system a pressure peak will occur due to the fast rising temperature leading to a higher pressure difference between reactor and environment and a lower pressure difference between reactor and fuel line. This is leading to oscillations in the total gas mass in the reactor which in turn are effecting the combustion process.

D. Numerical issues

The resulting system of differential equations is locally showing negative eigenvalues with high magnitudes, so an implicit ODE solver has to be used. In an implicit calculation scheme the problem $x_{k+1} = g(x_k, x_{k+1}, u_{k+1})$ has to be solved in every iteration step. For a nonlinear model the iteration function $g$ is nonlinear as well, so the solution of a nonlinear system of equations has to be calculated in every iteration step. Currently Matlab’s ODE15s is used to solve the differential equations. Since its performance depends largely on accurate jacobians of the used model function exact derivatives with respect to input and states should be supplied to the solver. Jarmolowitz [6] made use of numerical differentiation to get the needed derivatives. However, due to the numerical properties of the model this leads to high calculation effort even for quite inaccurate derivatives. To avoid these problems, analytical differentiation of the model is applied in this work.

IV. MODEL PREDICTIVE CONTROL

To stabilize the combustion process a Model Predictive Control (MPC)[[1]] is used. Starting from the current state of the controlled system, the MPC is calculating a prediction using the given model over a specified prediction horizon. The values for the manipulated variables are calculated as the result of a mathematical optimization of the prediction result by minimizing a specified cost function with respect to applied constraints.

A. Applied MPC Scheme

Due to the high nonlinearity of the model a nonlinear simulation is performed to predict the system behavior under the current input conditions. The effect off changed input conditions on the next system state is then expressed using a linear correction term. The result is a compromise between the low calculation effort of a linear MPC and the accuracy of a full nonlinear MPC.

1) Prediction of System Behavior: As a first step the system behavior under current input conditions is predicted by solving

$$\dot{X} = f(X, \Omega)$$

applying an implicit ODE solver. From the quasi-continous result the discrete states

$$x_k = X(t_0 + k \cdot T_s)$$

are picked, with $T_s$ denoting the sampling time of the MPC.

During the prediction process the jacobians of the model equation (5) are calculated so a linearization of (5) at the selected operation point $(X_0, U_0)$ is available without further calculation effort, it yields

$$\dot{x} = A \cdot x + B \cdot u + f(X_0, U_0)$$

with the deviation variables $x$ and $u$, defined by

$$x = X - X_0, \quad u = U - U_0.$$  

2) System Behavior with changed Input: A zero order hold discretization according to [13] results in the discrete state space model

$$\tilde{x}_{k+1} = A \tilde{x}_k + B \tilde{u}_{k-1} + f_k + B_k \Delta u_k$$

with the affine term $f_k$ and the output equation

$$y_k = [1, 0, ..., 0] \cdot x_k.$$  

Since a nonlinear prediction of $x_k$ is available from step one instead of (18)

$$\tilde{x}_{k+1} = x_{k+1} + B_k \Delta u_k + f_k$$

is used to predict the system behavior under changed input conditions.

3) Cost function, bounds and constraints: The cost function is selected as

$$J(\Delta u) = \sum_{i=1}^{H_p} \|y_{k+i} - r_{k+i}\|_Q^2 + \sum_{i=0}^{H_u-1} \|\Delta u_{k+i}\|_R^2 + \|y_{k} + H_p \|_Q_f.$$  

with weighting matrices $Q$, $Q_f$ and $R$, the reference trajectory $r$ and $y_k$ evaluated by (19), $H_p$ is denoting the prediction horizon, the length of the manipulating horizon is given by $H_u$.

The values of the manipulated variables are then determined by calculating

$$\min_{\Delta u} J(\Delta u)$$
subject to the actuator limits given by

\[ 500K < \ T_{in} < 700K \]  
\[ 0.4s < \ \tau < 1s \]  
\[ 0.5 < \ \phi < 10 \]  
\[ 0.2 < \ \phi < 5 \]

and

\[ |\Delta T_{in}| < 20K \]  
\[ |\Delta \tau| < 0.3s \]  
\[ |\Delta \phi| < 0.3 \]  
\[ |\Delta d| < 0.5 \]

using the solver package qpOASES [15].

Due to the sensitivity of the system a good control result could only be obtained reducing the weighting of input deviations and focusing on minimizing deviations in the controlled variable. Several different structural approaches for \( Q \) were tested, the best result was obtained by simply setting

\[ Q = I \] and  
\[ R = \lambda Q \] with \( 10^{-5} < \lambda < 10^{-2} \).

The use of a final constraint within this MPC resulted in unfeasibility of the underlying optimization problem, which leads to a relaxation of the constraint by the used optimizer. To avoid the computational overhead the final constrained was replaced by final costs, expressed by \( Q_f \). When \( Q = I \), numerical experiments resulted in an optimal value of \( Q_f = 100 \). Due to the complexity of the system a detailed stability analysis is still an unsolved problem.

\[ \text{Fig. 5. Simulation results of JSR controlled by MPC} \]

\[ \text{Fig. 6. Simulation results of JSR controlled by MPC} \]

\[ \text{B. Results} \]

Figure 5 shows a simulation result of the JSR being controlled by the presented MPC using an exact model for the observer, the corresponding input values are shown in figure 6. The simulation starts with the oscillating limit cycle. When the controller is switched on at \( t = 1s \) a small overshoot occurs, after which the JSR temperature is following the reference value with neglectable deviation to the reference. Although the reactor temperature is constant after \( t = 1s \), the changing input variables show that the reactor is not at a steady condition until \( t \approx 3s \). During this interval a steady chemical state is obtained without a large influence on the reactor temperature, so temperature alone is not sufficient for determining the current state of combustion.

After the input values reaches a steady state at \( t = 3s \), the reference value is set to \( T_r = 640K \). Due to the very high dynamics of the system, the reactor temperature is following the step with small deviations, again showing overshooting. When the steady state is again reached the reference value is changed to \( T_r = 620K \). Again the reactor temperature follows the reference very closely. At \( t = 7\text{sec} \) the reference value performs sinusoidal oscillations to demonstrate the dynamical abilities of the controller. In the first period the JSR shows some significant overshoot, indicating that the chemical steady state reached at \( T_r = 620K \) reacts very sensitive to temperature changes. However, the resulting instabilities are damped out by the controller through strong actuation of \( \phi \). During the next periods no chemical steady state is allowed to establish, so the reactor is following the reference trajectory without instabilities, further oscillations or significant overshooting.

However, the assumption of no model errors does not hold when the MPC should be applied to the real system. Regarding the experimental setup it is of significant interest if the used set of sensors is sufficient for stabilizing the JSR.

The results shown in figure 7 were obtained during simulations including the extended Kalman filter to reconstruct the full state signal. As model mismatch the heat transfer coefficient of the reactor hull in the simulation model was reduced by 20% compared to the model used in MPC and filter, since it is the system parameter with highest uncertainty. Figure 7 shows the simulation results when only the reactor temperature and the cumulated concentrations of all carbon hydrogens can be measured. As shown in figure 7 (Top) the MPC is not able to stabilize the reactor,
it continues to oscillate. Although the systems temperature and CH-signal is perfectly met by the observer, the internal observer states are showing a large mismatch compared to the states of the simulated system. This indicates that the system is not observable in the simulated setup and in consequence the MPC is failing to stabilize the reactor system.

To fix this problem two additional real-time capable sensors can be added to the reactor system. By analyzing chemiluminescence and infrared absorption the concentrations of $OH$ and $HO_2\cdot C_2H_5OCHO$ can be directly measured. The simulation results of the extended system are shown in figure 8. With the additional sensors the observer is able reproduce a state vector which is enabling the MPC to stabilize the reactor.

V. CONCLUSIONS AND FUTURE WORK

A. Conclusions

An analytical model for a jet stirred reactor using a full chemical reaction scheme has been presented. Based on this model a semi-linear MPC as well as an extended Kalman filter were implemented to stabilize a jet stirred reactor at an unstable working point. It was demonstrated that in general the system is controllable by an model predictive controller with good control results. If applied to the experimental setup the unavoidable model errors will spoil the observability with the currently applied sensors. It was shown that the result could be removed by adding two additional real-time capable sensors.

B. Future work

Since the main focus of this work is the use of a MPC on the described system, an extendet Kalman-Filter (EKF) was used as a simple and easy to implement observer. For several reasons the EKF is not well suited for this problem. A more advanced observer has to be used, e.g. of Kalman-Bucy or receding horizon type.

ACKNOWLEDGMENTS

The authors gratefully acknowledge the contribution of the Deutsche Forschungsgemeinschaft through the Collaborative Research Center 686 ”Model-Based Control of Homogenized Low-Temperature Combustion”.

REFERENCES