Model Reduction and Control of a Compressible Channel Flow with Combustion *

Lorenz Pyta∗ Mathias Hakenberg∗ Dirk Abel∗

Abstract: A model reduction for a compressible flow with combustion is performed using
the POD-Galerkin procedure. The model parameters are determined by an optimization. The
obtained reduced-order model is incorporated in a model predictive controller and results are
shown from a closed-loop CFD-simulation. The controller influences the fuel mass-flow boundary
condition to control the temperature at a certain point within the computational domain.

1. INTRODUCTION

In many types of combustion processes, e.g. a combustion in a rotary kiln for cement production, it is important
to guarantee a constant temperature profile over time. This will be hard to achieve if the fuel mass flow for the
combustion has a changing heat value. This may occur if waste is used for the combustion in order to reduce the
use of expensive fossil fuels. Thus a controller is needed to keep the temperature profile constant.

Modeling this types of combustion processes requires the consideration of the spatial extension of the system states.
Systems with non-negligible spatial dimension are called distributed parameter systems and are typically modeled
with partial differential equations (PDEs) e.g. the Navier-Stokes-Equations for flow problems. However, designing
a feedback controller requires low dimensional models of ordinary differential equations (ODEs). One established
approach to retrieve an ODE-Model from a PDE is the Proper Orthogonal Decomposition (POD) and subsequent
Galerkin projection (see e.g. Holmes et al. [1996]). The idea is to compute a set of spatial basis functions of a subspace
containing most information from empirical data and to project the PDE onto this subspace to arrive an ODE.

These methods have been applied in many different cases of flow control. Kunisch and Volkwein [1999] obtained
a reduced model for the Burgers Equation via POD-Galerkin technique. The empirical data for building up the
model has been generated from simulations. Baker and Christofides [1999] analyzed the incompressible two-
dimensional Navier-Stokes equations in order to describe Newtonian fluids and to synthesize a nonlinear controller.
The actuation has been realized via a volume force in the

simulations needed to obtain the data for the POD. However, combustion processes like all processes with noteworthy temperature changes, require compressible modeling. An investigation of the two-dimensional compressible Navier-Stokes-Equations has been given by Iollo et al. [2000]. They formulated a compressible Galerkin-model with conservation equations in velocity, pressure and specific volume. Heat flow was not considered. The choice of specific volume instead of density guarantees a polynomial structure of the model. A compressible case is also covered in Gloerfelt [2008]. The POD is applied in order to describe flow oscillations in a cavity. Again the specific volume is chosen as value for the conservations equations and the Galerkin projection. Some additional techniques for compressible POD have been introduced by Rowley et al. [2004]. They used simplified isentropic but compressible Navier-Stokes equations for the Galerkin-projection and modified the inner product for the projection in order to respect both thermodynamic and kinematic variables. An approach to include actuation via changing boundary conditions in the reduced order model was outlined by Graham et al. [1999]. They introduced an additional mode, which homogenizes the given data ensemble at every time step and thus represents the boundary conditions. The POD-Galerkin method delivers the structure of the model and the corresponding coefficients of the model. As the computation of the modes requires empirical data of the process, the calculation of the coefficients depends on the modes and their derivatives, which can lead to numerical problems. In order to improve the accuracy of the reduced models, Couplet et al. [2005] and also Cordier et al. [2009] calibrated the coefficients of the model using optimization methods and regularizations.

In the present paper the outlined knowledge is combined to receive a reduced model via the POD-Galerkin method for a compressible channel flow with combustion. For that purpose the models in Gloerfelt [2008] are expanded with a combustion term to consider the heat flow. Actuation via boundary conditions is considered using the ’control function’ approach of Graham et al. [1999]. The model is calibrated with the tools introduced in Cordier et al.

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A model predictive controller is set up using the reduced model to control the temperature inside the channel at a specific point. Section 2 introduces the plant. Section 3 gives a short overview over the POD-Galerkin method, while the actual reduced order model is derived in Section 4. The controller design is described in Section 5 connected with the investigation of the controller’s performance. Section 6 gives a short conclusion.

2. SIMULATION AND PLANT

The plant considered in this paper is a compressible channel flow with combustion simulated with the CFD-Solver Fluent from ANSYS [2011]. In order to simplify computations and to utilize symmetry, the upper half of a longitudinal cut through a channel of 50 m length and a height of 5 m is considered as plant. Thus the computation area is two-dimensional with a length of 50 m and a height of 2.5 m. For further modeling only two dimensions have to be taken into account.

The fuel inlet with a height of 12.5 cm, where methane enters the channel with a constant temperature of 300 K, is located on the lower part of left boundary. The mass flow of methane is variable and can be actuated by the controller. Preheated air with a mass flow of 21.6 kg/s enters the channel at a constant temperature of 973 K through the upper part of the left boundary. The velocity vanishes on the walls along the channel and heat transfer across the wall is also considered. On the right side of the channel a pressure outlet condition with a gauge pressure of 1 bar is used.

A sketch of the plant is shown in Fig. 1.

![Fig. 1. Boundary conditions of the plant](image)

The physics of the channel-flow are described by the conservation of mass, conservation of momentum and conservation of energy. The equation for conservation of mass can be written as

$$\frac{\partial}{\partial t} \rho + \text{div}(\rho \mathbf{v}) = 0$$

for the whole system and (without concerning mass diffusion)

$$\frac{\partial}{\partial t} (\rho Y_k) + \text{div}(\rho Y_k \mathbf{v}) = \dot{\omega}_k$$

for every species, where \(\rho\) denotes the density, \(\mathbf{v}\) the velocity, \(Y_k\) the mass fraction of species and \(\dot{\omega}_k\) the generation rate of species \(k\). Further the reaction of species is described by

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O.$$  

The conservation of momentum becomes with \(\mathbf{v} = (v_1, v_2) = (u, v)\) in streamwise direction \(x_1\) and

$$\frac{\partial}{\partial t} (\rho \mathbf{v}) + \text{div}(\rho \mathbf{v} \mathbf{v}) = -\frac{\partial p}{\partial x_1} + \tau_{11} + \tau_{21}$$

in normal direction \(x_2\). In these equations \(p\) denotes the pressure and \(\tau_{ij}\) the stress tensor computed by

$$\tau_{11} = \mu \left( \frac{4}{3} \frac{\partial \mathbf{u}}{\partial x_1} \cdot \mathbf{v} - \frac{2}{3} \frac{\partial \mathbf{v}}{\partial x_1} \right)$$

$$\tau_{22} = \mu \left( \frac{4}{3} \frac{\partial \mathbf{u}}{\partial x_2} \cdot \mathbf{v} - \frac{2}{3} \frac{\partial \mathbf{v}}{\partial x_1} \right)$$

$$\tau_{12} = \tau_{21} = \mu \left( \frac{\partial \mathbf{u}}{\partial x_2} \cdot \mathbf{v} + \frac{\partial \mathbf{v}}{\partial x_1} \right)$$

with the dynamic viscosity \(\mu\).

In order to close the system of equations the ideal gas law

$$p = \rho RT$$

is applied. Here \(R\) denotes the specific gas constant and \(T\) the temperature of the gas. For the caloric state equation \(e = c_v T\)

Finally, the conservation of energy is described by

$$\frac{\partial (\rho(e + \frac{\|\mathbf{v}\|^2}{2}))}{\partial t} + \text{div}(\rho(e + \frac{\|\mathbf{v}\|^2}{2}) \mathbf{v}) = - \text{div}(\mathbf{v} p)$$

$$+ \Delta (kT) + \rho \dot{q} - \sum_{k=1}^{N} h_k \dot{\omega}_k + \sum_{i,j=1}^{2} \frac{\partial (\tau_{ij} v_i)}{\partial x_j}$$

with \(\dot{q}\) as the volumetric heat flow, the enthalpy of formation \(h_k\) and the thermal conductivity \(k\).

These equations are solved by the CFD-Solver Fluent using an implicit pressure based solver with a Courant number of ten and a cell-based least square method to approximate the gradient. For turbulence the \(k-\epsilon\)-model was applied. The effects of radiation are considered using the P1-model. The input of the plant is the mass-flow of methane into the channel scaled with the nominal value 3 kg/s. The controlled variable is the cell average of the temperature at the position (20 m, 1.2 m).

For the model reduction dynamic information about the plant is needed in form of snapshots. These snapshots contain the data of different physical variables on the whole computational domain at certain points in time. To generate this snapshot-data the plant is simulated over a time scale of 15 s with a step size of 0.1 s for the data export. The 151 snapshots include all values of density, pressure, velocity and of mass-concentration of oxygen and methane. To generate dynamic information the plant has been simulated with an excitation of the left boundary condition. Fig. 2 shows the fuel mass flow at the inlet as a function of time. The mass-flow is scaled with the nominal value 2.5 kg/s and time is scaled by the cycle time.

3. REDUCED-ORDER-MODELS

The derivation of a reduced-order-model for a given plant with POD-Galerkin consists of two steps. The first is to compute a set of spatial basis functions via proper
orthogonal decomposition based on the snapshot-data, which should cover the operating range of the system. Second the investigated PDE is reduced to a system of ODEs by application of the Galerkin-projection. Some theoretical background for the POD and the Galerkin-projection is outlined in paragraph 3.1 and 3.2. The model-reduction for the present case is presented in Section 4.

3.1 Proper Orthogonal Decomposition

Given a data set $y(t, x)$. The goal of the POD is to decompose the data into temporal coefficients $a_i(t)$ and spatial functions $\varphi_i(x)$ such that

$$ y_N(t, x) = \sum_{i=1}^{N} a_i(t) \varphi_i(x) $$

is the optimal approximation of $y(t, x)$ in a time-averaged least-squares sense (see e.g. Holmes et al. [1996]). This problem leads to the determination of the spectrum of a linear, self-adjoint and compact operator. In case of time-discrete data and applying the method of snapshots introduced by Sirovich [1987] the solution simplifies to the calculation of eigenvalues of a correlation matrix. Let $\langle \cdot, \cdot \rangle$ be a spatial inner product in $L^2(\Omega)$ and $N_t$ the number of time-steps in the data. Then the $(N_t \times N_t)$ correlation matrix can be computed by

$$ C_{ij} = \langle y(t_i, x) y(t_j, x) \rangle. $$

The temporal coefficients $a_i(t)$ are determined as eigenvectors to the largest eigenvalues of $C$, hence

$$ C a_i = \lambda_i a_i. $$

The POD modes $\varphi_i(x)$ are given via projecting $a_i$ on the data set $y$ by

$$ \varphi_i(x) = \frac{1}{\sqrt{\lambda_i}} a_i(t)^T y(t, x). $$

This computation ensures that the POD modes form an orthonormal basis of an optimal subspace of $L^2(\Omega)$. In the case that $y(t, x)$ is multi-dimensional the sum of the inner products of the different dimensions of $y$ leads to the same result. For the compressible model reduction, different physical quantities like velocity or pressure need to be combined in one inner product. Therefore a proper scaling of the variables is essential to receive a meaningful decomposition. Here all variables will be scaled by the operating point values. So $y(t, x)$ has been scaled with the average values of the initial simulation. The calculation of POD modes ensures a model of low dimension and optimal representation of the ensemble data.

3.2 Galerkin-Projection

With this modal decomposition into temporal coefficients $a_i(t)$ and spatial basis functions $\varphi_i(x)$ a transformation of the PDE into a system of ODEs can be achieved. Substitution of the series expansion (10) into the PDE and projecting the residual onto the $j$-th basis function results in an ODE for the $j$-th temporal coefficient $a_j$. Repeating this procedure for each of the temporal coefficients gives a system of $N$ ODEs. The corresponding calculation is the following: Given a PDE with the structure

$$ \dot{y}(t, x) = f(y, \partial_t y, \ldots, \partial_t^n y). $$

From the Orthogonal Decomposition follows

$$ y(t, x) \approx \sum_{i=1}^{N} a_i(t) \varphi_i(x) \quad \text{and} \quad \langle \varphi_i(x), \varphi_j(x) \rangle = \delta_{ij}, $$

where $N$ is the number of POD modes. Then also the identity

$$ \dot{a}_j = \langle \dot{y}(t, x), \varphi_j(x) \rangle $$

$$ \approx \langle f \left( \sum_{i=1}^{N} a_i \varphi_i, \sum_{i=1}^{N} a_i \partial_t \varphi_i, \ldots, \sum_{i=1}^{N} a_i \partial_t^n \varphi_i \right), \varphi_j \rangle $$

$$ = \tilde{f} (a, \varphi, \partial_t \varphi, \ldots, \partial_t^n \varphi) $$

holds. Boundary conditions do not explicitly occur in the resulting ODE-system. Thus for an exact matching of the boundary conditions, the boundary conditions have to be satisfied by the POD modes. This will only be the case for homogeneous boundary conditions, since the POD modes inherit these conditions from the data set and all linear combinations will fulfill them too. Inhomogeneous boundary conditions can be satisfied with additional modes introduced by Graham et al. [1999]

$$ y(t, x) = y_h(t, x) + \tilde{y}(t, x) + u(t) \tilde{y}(t, x). $$

Thereby $\tilde{y}(x)$ meets the stationary boundary conditions while $y_h(x)$ represents the influence of the time dependent boundary condition $u(t)$. The POD is applied just on $y_h(t, x)$ and so these modes meet the homogeneous boundary conditions of $y_h(t, x)$. Thus the modes of $y_h$ combined with $\tilde{y}(x)$ and $\tilde{y}(x)$ fulfill the inhomogeneous boundary conditions.

The additional modes $\tilde{y}(x)$ and $\tilde{y}(x)$ are in general not orthogonal to the POD modes of $y_h$ and the equations are modified to

$$ \dot{a}_j(t) = \langle \sum_{i=1}^{N} \tilde{a}_i(t) \varphi_i(x), \varphi_j(x) \rangle - \dot{u} \langle \tilde{y}(x), \varphi_j(x) \rangle $$

$$ \sum_{i=1}^{N} a_i(t) \varphi_i(x) + \tilde{y}(x) + u(t) \tilde{y}(x) = \sum_{i=1}^{N+2} a_i(t) \varphi_i(x). $$

Because the input variable $\dot{u}$ appears as time-derivative in (18), its more convenient to choose

$$ w = \dot{u} $$

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as input of the system. The resulting model is a system of ODEs for the temporal coefficients $a_j(t)$ related to modes $\varphi_j(x)$ containing most information of the system dynamics. The $j$-the ODE of the model describes the change of the influence, that the mode $\varphi_j(x)$ has on the solution.

4. MODEL-REDUCTION OF THE CHANNEL-FLOW

At first some additional equations not directly included in the CFD-Simulation but needed for the reduction are presented. Together with the equations for the plant this results in a system of nonlinear PDEs, which will be reduced with the presented methods to a system of ODEs. Because direct calculation of the coefficients of the ODEs is ill conditioned, the structure of the reduced-order-model will be maintained, but the coefficients will be determined indirectly by an optimization.

4.1 Additional equations for the channel-flow

First methane (equivalent to $k = 1$), oxygen ($k = 2$) and $CO_2 + 2H_2O$ ($k = 3$) are chosen as species for equation (2) and (3). Further the kinetics of the reaction shall follow the differential equations

$$\frac{\partial}{\partial t}(\rho Y_1) = -k_R \rho Y_1 \rho Y_2$$

$$\frac{\partial}{\partial t}(\rho Y_2) = -k_R \rho Y_2 \rho Y_1,$$

where $k_R$ is the rate constant. The change of the rate constant due to changes in temperature are described by the Arrhenius ansatz, which presumes an exponential relation. The effects of radiation are described via the Stefan-Boltzmann law

$$\dot{q} = \frac{1}{V} \epsilon \sigma AT^4$$

with the variables $\epsilon$ as the emissivity, $\sigma$ the Stefan-Boltzmann constant and surface and volume $A$ and $V$. Together with the equations (1) - (8) these form a system of nonlinear PDEs.

4.2 The reduced ODE-model

A direct Galerkin projection of the nonlinear PDEs into a reduced order model would lead to a model with terms of high order owing to the $T^4$-Term due to radiation and the $e^T$-Term due to the Arrhenius ansatz for the reaction coefficient. Also many physical quantities have to be taken to account. With the assumption that $k$ and $R$ are constant, and via a linearization of the equation around a temperature working point $T_0$, the structure of the model can be simplified to an ODE-System with quadratic structure and only six physical quantities. These are the specific volume $\xi$, the streamwise and normal velocity $u$ and $v$, the absolute pressure $p$ and the mass concentrations of fuel ($\chi = \rho Y_1$) and oxygen ($\psi = \rho Y_2$). The choice of the inverse density (see Gloorfeld [2008]) ensures the polynomial structure of the resulting model, because the temperature can be written as $RT = \rho \xi$. With the choice of

$$y(t, x) = (\xi \quad u \quad v \quad p \quad \psi \quad \chi)^T = (y_1(t, x) \ldots y_{VI}(t, x))^T$$

and the dot product

$$\langle y(x), \varphi(x) \rangle = \sum_{i=1}^{VI} \langle y^i(x), \varphi^i(x) \rangle$$

the resulting model has the structure

$$\dot{a}_j = a^T (\Xi^j + U^j + V^j + D^j + \Psi^j + X^j) a + w g_j$$

$$\dot{a}_{N+1} = 0$$

$$\dot{a}_{N+2} = w.$$
Fig. 3. Comparison of the projected and the model based coefficients for the whole simulation-time validation samples. With four modes more than 90% of the relative information content of the snapshot ensemble can be represented. This number of modes is used for the reduced order model. Together with the time average flow field mode and the actuation mode, the reduced order model comprises six states in total. The Fluent simulation has over seven million states.

5. CONTROLLER-DESIGN AND PERFORMANCE

After the derivation of a reduced model for the given plant, it is possible to design a model predictive controller, which explicitly uses this model.

5.1 Controller and Estimator

The controller solves a finite horizon open-loop control problem in every time step and applies the first value of the calculated optimal control sequence to the plant. For that purpose the nonlinear continuous time model is linearized and discretized in each time step. To take advantage of the available continuous time description of the plant, the free system response is predicted using the full nonlinear model. To secure stationary accuracy the error in the prediction at the point of measurement $d_0 = y - y_{pred}$ is fed back. The reference trajectory is shifted with this value so that

$$\text{ref} + d_0 - y = \text{ref} + (y - y_{pred}) = \text{ref} - y_{pred}$$

(27)

holds. In this formulation the minimum of $\text{ref} - y_{pred} - d_0$ (the predicted output and the shifted reference trajectory) leads to a minimum of $\text{ref} - y$, which is the desired goal of the control. Since the model predictive controller needs the state of the system an estimator was implemented in addition. To unify the time continuous plant with the discrete output and input variables a hybrid extended Kalman filter (see e.g. Simon [2006]) was used. The estimation problem could be solved using only the controlled variable (temperature at $(20\ m, 1.2\ m)$) as measurement.

5.2 Results

This controller has been tested in a closed loop simulation using the CFD simulation as plant. As the controller has been implemented in Matlab, a coupling of Matlab with the CFD-Solver Fluent has to be designed as closed-loop interface. This has been done using the possibility to change boundary conditions in Fluent via a user defined function (udf). Matlab generates after every time step a new file containing this udf with the new boundary conditions computed by the controller. Fluent is run as batch process in Matlab and simulates the plant with the new boundary condition one time step and hands the measurement information, that is the temperature value at the position $(20\ m, 1.2\ m)$, to the controller.

In order to evaluate the performance, the controller has been analyzed regarding reference action and disturbance rejection. The measurement of this output has been disturbed with a white measurement noise with $\sigma = 0.1\ K$. The reference trajectory ranges from $1800\ K$ to $2050\ K$, which doubles the operating range from $1925\ K$ to $2050\ K$ covered by the data used for training the model. In spite of the big range the controller was able to follow the reference as shown in Fig. 4.

Fig. 4. Time response for varying reference trajectory

Second the controller received an stationary reference value. Then the mass flow inlet has been increased by 20% as an unknown disturbance. This perturbation is neither known to the controller nor to the model, because it did not occur in the snapshots. But the controller has the ability to compensate the disturbance as shown in Fig. 5. The corresponding values for the input of the plant are shown in Fig. 6. The values are scaled with the factor $2.5\ kg/s$, so that the maximum change of the input is roughly $1.2\ kg/s$. The amplitudes are in an acceptable range regarding the amplitude of the disturbance. The shown values are not the input variable to the model $w$, but the value of the boundary condition $u$.

6. CONCLUSION AND OUTLOOK

The applied procedure is able to produce a reduced model for the model predictive controller, which is good enough to enable a good controller performance. Due to the POD-Galerkin procedure the polynomial order of the model is known and the number of states is small. This allows an optimization of the model coefficients to receive an accurate model. Drawbacks are, that the model only
To compute the Matrix $\Xi_j$ first the related ODE has to be set up. With the notation $\frac{\partial}{\partial r_1} = \partial_1$ and $\frac{\partial}{\partial r_2} = \partial_2$

$$\xi = \left( \frac{1}{\rho} \right) = -\frac{\rho}{\rho^2} = \frac{1}{\rho^2} (\rho \partial_1 u + \rho \partial_2 v + u \partial_1 \rho + v \partial_2 \rho)$$

$$= \xi \partial_1 u + \xi \partial_2 v - u \partial_1 \xi - v \partial_2 \xi. \quad (A.1)$$

follows. Using (19), (23) and (24) further

$$\langle \xi, \varphi_j \rangle = \langle \xi \partial_1 u + \xi \partial_2 v - u \partial_1 \xi - v \partial_2 \xi, \varphi_j \rangle$$

$$= \langle \sum_{i=1}^{N+2} a_i \varphi_i^{\prime \prime} + \sum_{k=1}^{N+2} a_k \partial_1 \varphi_k^{\prime \prime} + \sum_{k=1}^{N+2} a_k \partial_2 \varphi_k^{\prime \prime}, \langle \sum_{i=1}^{N+2} a_i \partial_1 \varphi_i^{\prime} + \sum_{k=1}^{N+2} a_k \partial_1 \varphi_k^{\prime}, \varphi_j \rangle \rangle$$

$$= \left( a_1 \cdots a_{N+2} \right)^T \left( \Xi_{ik} \right)_{ik} \left( a_1 \cdots a_{N+2} \right)^T = a^T \Xi^T a$$

holds with

$$\Xi_{ik} = \langle \xi \partial_1 \varphi_i^{\prime \prime} + \xi \partial_2 \varphi_i^{\prime \prime} - \partial_1 \varphi_i^{\prime \prime}, \varphi_k^{\prime \prime} \rangle$$

An ODE for the coefficient $a_j$ is gathered via the equation

$$\langle \dot{a}_j, \varphi_j \rangle = \langle \sum_{i=1}^{N+2} \dot{a}_i \varphi_i, \varphi_j \rangle = \dot{a}_j + \langle \sum_{i=1}^{N+2} \dot{a}_i \varphi_i, \varphi_j \rangle = \dot{a}_j - w g_j$$

$$= \langle \dot{\xi}, \varphi_j \rangle + \cdots + \langle \dot{\chi}, \varphi_j \rangle.$$

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Appendix A. EXEMPLARY COMPUTATION FOR THE REDUCED MODEL