Adjoint-based Variational Data Assimilation for the Analysis of an Experimental Pulsed Detonation Combustor with a Compact Shock-focusing Geometry

M. Lemke, J.A.T. Gray, J. Reiss, J.P. Moeck and J. Sesterhenn
Institute of Fluid Dynamics and Technical Acoustics, Technische Universität Berlin
Berlin, Germany

1 Research Rational

Pulsed detonation combusters (PDC) promise higher efficiency compared to isobaric combusters, which are presently used in stationary gas turbines and aero engines. The core idea is to use the thermodynamic advantages of an isochoric cycle. However, in order to directly initiate the detonation, a large amount of energy is required. Therefore, the combusters usually make use of the deflagration-to-detonation transition. In general, the fluid mechanical processes in the chamber are difficult to analyze, due to the inherent measurement restrictions of a detonative flow regime.

The aim of this work is to analyze the experimental data of a PDC with an alternative method of obtaining DDT. Time-resolved pressure measurements serve as the target for an adjoint-based variational data assimilation. An optimal one-dimensional description of the process governed by the reactive Navier–Stokes equations is derived. The parameters of the employed Arrhenius chemistry model and flow parameters are adapted. This is important because once the numerical simulation data match those of the experiment, other quantities, such as velocity and temperature, can be extracted from the numerical solution.

2 Methodology

Experimental Configuration

The experimental configuration under consideration is a detonation chamber, which is operated in single-shot mode. The tube is filled with hydrogen and oxygen-enriched air. A deflagration is ignited by a standard spark plug. The transition to detonation occurs due to the focusing of reflected pressure waves near a convergent-divergent nozzle. For the measurements, the tube is equipped with numerous flush-mounted pressure sensors, which are sampled at 1 MHz.

Correspondence to: mathias.lemke@tnt.tu-berlin.de

Numerical Model

The reactive compressible Navier–Stokes equations for one dimension with variable area F are given by

$$\partial_t \varrho F + \partial_x \varrho F u = 0 \tag{1}$$

$$\partial_t \varrho F u + \partial_x \left(\varrho F u u + F p\right) = p \partial_x F + \partial_x F \tau \tag{2}$$

$$\begin{aligned} \partial_t \varrho F e_s + \partial_x \left(u \varrho F e_s + p F u\right) - u F \partial_x p + F \sum_{k=1}^{N} \Delta h^o_{f,k} \dot{\omega}_k \\ = F \tau \partial_x u + \partial_x F u \tau + \partial_x \left(F \lambda \partial_x T\right) \end{aligned} \tag{3}$$

$$\partial_t \varrho F Y_k + \partial_x \varrho F u Y_k - F \dot{\omega}_k = \partial_x \left(F \varrho D_k \frac{W_k}{W} \partial_x X_k \right). \tag{4}$$

Therein, ϱ denotes the density, u the velocity, e_s the inner (sensible) energy, p the pressure, τ the viscous stress tensor, W the mean molecular weight, Y_k the mass fraction of species k of N, and X_k the mole fraction. The coefficients λ and D_k are the heat and species diffusion coefficients. $\Delta h^o_{f,k}$ corresponds to the standard formation enthalpy. The reaction rate $\dot{\omega}_k$ is modeled by an Arrhenius approach without reverse reactions. The summation convention applies.

In order to enable a simple effective numerical representation of the experimental setup, the above system is simplified by various means. First, the viscous terms τ are neglected. Corresponding effects are partly represented by modified diffusion coefficients λ and D, which are controlled by the data assimilation procedure. In addition, the density is absorbed into the species constant $\bar{D} = \varrho D$. The temperature dependence of the specific heat is also neglected. The energy equation can be rewritten in terms of pressure, leading to more simple adjoint equations [1]. For the assimilation, only one-step chemistry is considered. Furthermore, only one effective species Y with $\nu' = 1$, varying from one (unburned) to zero (burned), is used. The effective experimental kinetics are covered by modification of the Arrhenius parameters A and E_a. The heat release results in $\dot{\omega}_T = FQ\dot{\omega}$, in which the constant Q is chosen in accordance with the considered mixture of hydrogen and oxygen-enriched air.

Numerical Implementation

The space discretization is realized by a finite difference scheme of fourth order. A one-dimensional grid with equidistant points is used. An adiabatic wall is applied at the left boundary and an outflow condition is applied at the right boundary. For the time discretization a standard Runge-Kutta scheme of fourth order is employed. The total number of time steps is defined by one convectional length of the reactive front.

Table 1: Selected parameters for the considered mixture of hydrogen and oxygen-enriched air.

γ	1.1775	[1]
R	8.3144	[J/mol/K]
W	0.0223	[kg/mol]
$C_v = \frac{R/W}{\gamma - 1}$	2100.5399	[m^2/s^2/K]
$Q = -\frac{\dot{\omega}_T}{\dot{\omega}}$	$6.2008 \cdot 10^6$	[m^2/s^2]

Since the direct and the adjoint equations are similar by means of structure, the same discretization is used for both sets. In order to ensure stable computations, implicit filters are applied for the direct and adjoint computations.

Adjoint Data Assimilation

To guide the reader through the intended adjoint-based data assimilation, the general procedure is sketched on an abstract level. As in [1], a matrix-vector notation is used. The vector space is the full solution in space and time.

The adjoint equations arise from a scalar value, the so-called objective function. It is defined by the integral difference between the numerical system state q and the experimental data q_{exp}

$$J = \frac{1}{2} \left(q - q_{\mathrm{exp}}\right)^T \left(q - q_{\mathrm{exp}}\right). \tag{5}$$

The system state itself is calculated under the constraint of the governing Navier–Stokes equations noted as

$$N(q, \alpha)q = 0, \tag{6}$$

with α as a free parameter. The goal of the assimilation is to modify the solution q by adaptation of the parameter α so that the numerical state matches the experimental data. A minimum of J is sought. If the objective function is non-linear, a linearized formulation must be derived. Linearization of J around a given base state $q = q_0 + \delta q$ leads to

$$\delta J = (\underbrace{q - q_{\mathrm{exp}}}_{g})^T \delta q. \tag{7}$$

Therein, the change of state δq is the solution of the linearized constraint, the Navier-Stokes equations linearized with respect to q_0 and α.

$$N\delta q + \underbrace{N q_0}_{f} \delta\alpha = 0 \tag{8}$$

In order to derive the adjoint equations, this constraint is added to the objective in a Lagrangian manner, using a multiplier q^*.

$$\begin{aligned} \delta J &= g^T \delta q - q^{*T} \underbrace{\left(N\delta q + f\delta\alpha\right)}_{=0} && (9) \\ &= \delta q^T \left(g - N^T q^*\right) - \delta\alpha^T (f^T q^*) && (10) \end{aligned}$$

By demanding that the adjoint state q^* is the solution of

$$g - N^T q^* = 0 \tag{11}$$

we obtain

$$\delta J = -\delta\alpha^T (f^T q^*). \tag{12}$$

The change of the objective becomes independent of the solution δq.

The expression $f^T q^*$ can be interpreted as the sensitivity of the parameter α on the objective, since

$$\frac{\delta J}{\delta \alpha} = -f^T q^* \tag{13}$$

holds. Thus, the adjoint solution can be used as gradient for the minimization of J.

According to the adjoint formalism, the set of governing equations (1)-(4) is to be linearized with respect to every primitive variable $q = (\varrho, u, p, Y)$ and the control parameters A, E, $\bar{D}$ and λ. It is assumed that the parameters are constant in terms of space and time. The linearized equations are added to the linearized objective function, defined by the experimental data, in a Lagrangian manner using $q^* = [\varrho^*, u^*, p^*, Y^*]$ as adjoint variables. Rearranging with respect to all independent variables, including partial integration, leads to the adjoint equations and gradient formulations for the mentioned parameters.

$$\begin{aligned} \delta J = \quad & \delta q^T \Big(g + A^T \partial_t q^* + B^T \partial_x q^* \\ + \quad & \underbrace{\hat{C}^T \partial_x C^T q^* - \tilde{C} \partial_x c + L^T q^* + N^T \partial_x M F \partial_x q^* \Big)}_{\text{adjoint equation}} \\ + \quad & \delta A \left[(-p^* Q + Y^*) \frac{F\omega}{A} \right] + \delta E_a \left[(p^* Q - Y^*) \frac{F\omega}{RT} \right] \\ + \quad & \delta \lambda \left[p^* \partial_x F \partial_x T \right] + \delta \bar{D} \left[Y^* \partial_x F \partial_x Y \right] \end{aligned} \tag{14}$$

3 Results

Based on an iterative procedure using the adjoint-based gradient information, an appropriate numerical model is found. The flow and Arrhenius parameters A, E, $\bar{D}$, and λ are adapted. The numerical solution matches the experimental data within the accuracy of the employed model and the measurement data, see Figs. 1 and 2. All results are normalized. Amplitudes and an extensive discussion on the results will be given on site.

4 Summary

A strategy to develop a reduced-order model (one-dimensional) of a pulse detonation combustor is presented. Experiments are used to adjust the parameters of the numerical modeling by means of an adjoint-based variational data assimilation procedure.

References

[1] M. Lemke, J. Reiss, and J. Sesterhenn, "Adjoint based optimisation of reactive compressible flows," *Combustion and Flame*, vol. 161, no. 10, pp. 2552 – 2564, 2014. [Online]. Available: http://www.sciencedirect.com/science/article/pii/S001021801400100X

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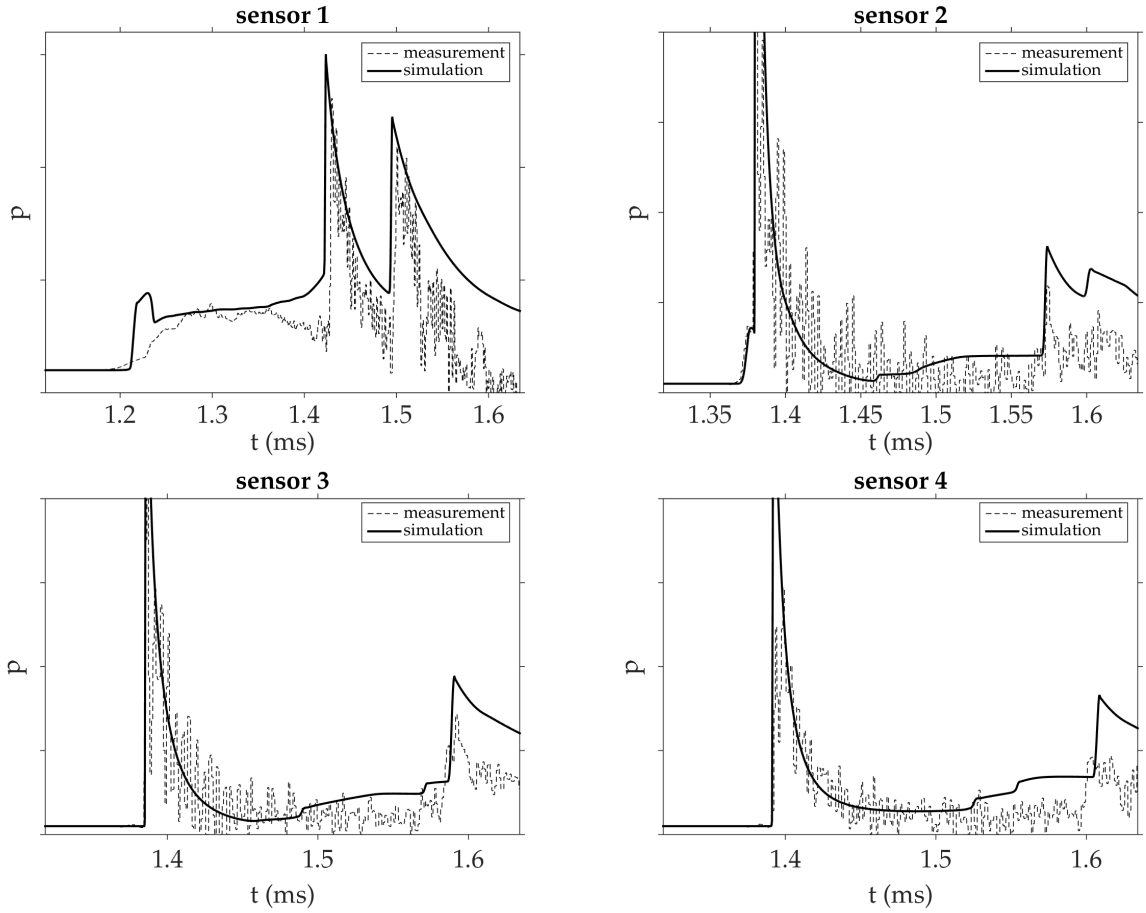

Figure 1: Pressure evolution of the adapted numerical simulation at the measurement positions, see Fig. 2(a). A very good agreement to the experimental data is found. The pressure signals match in terms of phase and amplitude.

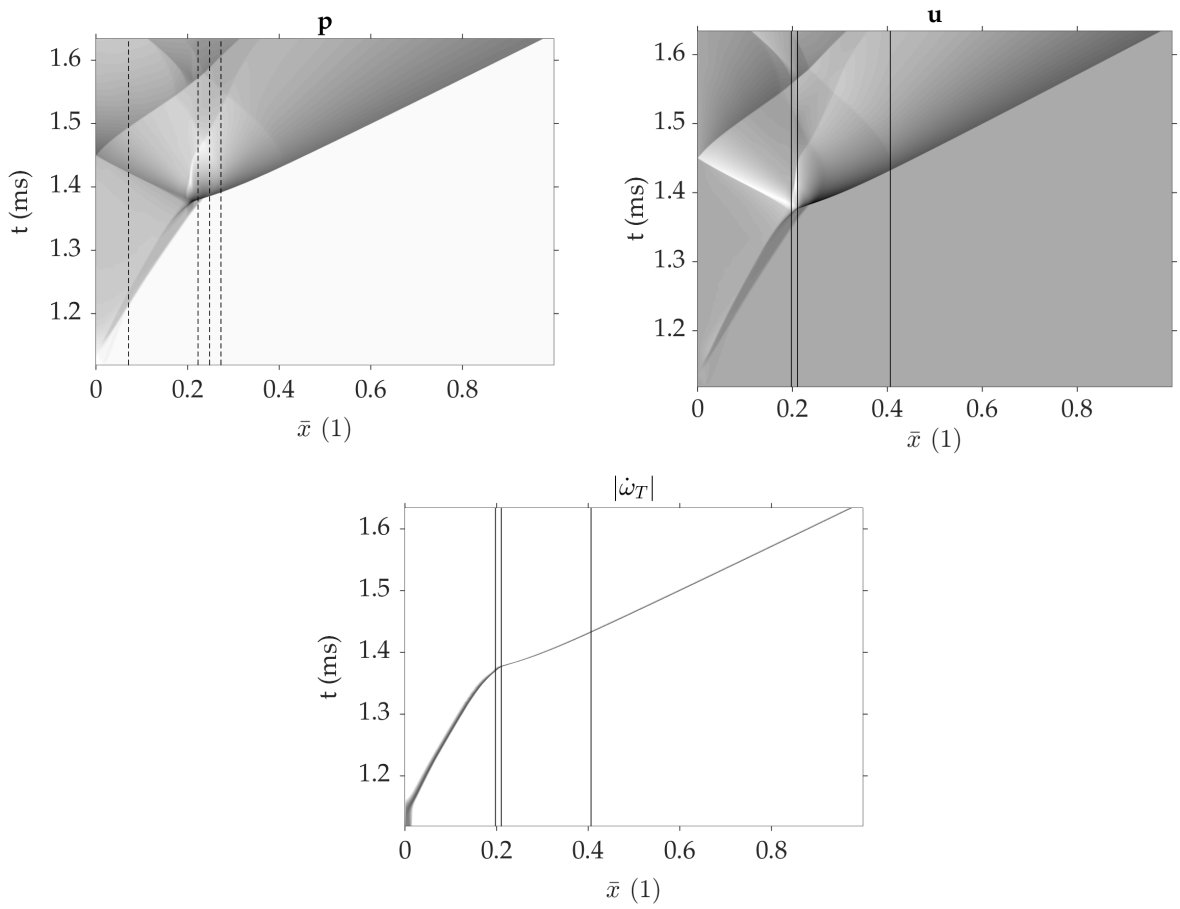

Figure 2: (a): Pressure p evolution in time and space, shown in logarithmic scale. The dashed lines correspond to the measurement positions. A strong compression is identified as well as a detonation, occurring near the narrowest cross section. Also a reflection of the detonation at the left wall is visible. (b): Velocity u evolution in time and space. The solid lines correspond to axial points where the geometry changes. Detailed information will be given on site. Two strong waves caused by the detonation are visible. The velocity indicates an over-driven detonation. (c): Total reaction rate in logarithmic scale. A supersonic combustion can be identified. *All spatial positions $\bar{x}$ are normalized with respect to the length of the computational domain.*