Computers and Mathematics with Applications 67 (2014) 1521–1544

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

Optimal control of the temperature in a catalytic converter

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ARTICLE INFO

Article history:
Received 26 August 2013
Received in revised form 6 February 2014
Accepted 8 February 2014
Available online 13 March 2014

Keywords:
Catalytic converter
Combustion
Exhaust pipe
Gas dynamics network
Optimization
Small Mach number

ABSTRACT

This paper is concerned with the optimization of the dynamics of the gas flow in an exhaust pipe. As a prototypical question the start up heating of the catalytic converter is considered. Reaching the optimal temperature in the converter rapidly competes against the costs, i.e., releasing too much unburnt fuel in the exhaust gases. The underlying model is a one dimensional small Mach number asymptotic gas dynamic model for a mixture of burnt and unburnt gases, formulated on a network consisting of the various pieces of the exhaust tube. For the optimization, adjoint calculus is applied on the continuous level. The resulting system is then discretized. Finally, numerical examples show the validity of this approach.

1. Introduction

The control and the reduction of the emissions caused by vehicles is, and has been, an import issue over the last 5 decades. The first restrictions were introduced by the government of California (USA) in the early 1960s. In 1970 the European Community passed first laws regarding exhaust gas pollution. Today, there is the *Euro* 5 standard and the next *Euro* 6 standard will be compulsory in 2014 in Europe. Many other countries nowadays use or introduce similar restrictions.

For the reduction of the concentration of CO, NO_x and C_xH_y in the exhaust gas, there is a classical technical solution, namely in most cases two catalytic converters are installed in the exhaust pipe system. The function of the catalytic converters depends strongly on the temperature in the converters. There is a lower limit (about 600 °C) for a good function and an upper limit to avoid damages. In particular, right after engine start there is a critical time interval where the temperature in the converters is not high enough. A method of heating after the engine start is the combustion of unburnt gas in the catalytic converters. Modern exhaust systems can control the ratio of oxygen and fuel in the combustion chamber of the engine. By choosing a ratio with more fuel and less oxygen some unburnt fuel flows to the catalytic converters where it can be used for an exothermic reaction. Clearly, there is a competition between reaching fast the optimal converter temperature and using very little unburnt fuel in the exhaust gas. This is the main issue in this paper. We show, how to compute an optimal inflow distribution of unburnt gas (into the exhaust tube) with respect to a cost function that will be presented below.

To face this problem, one has to model, appropriately, the gas dynamics in the exhaust pipe and the heat dynamics in the converters. In addition, we do not only need an appropriate model but also a model which allows fast direct simulations in order to be able to apply optimization tools, which typically need several simulations during the optimization. In this sense, this paper can be seen as a prototypical example for optimization in a compressible gas dynamic setting with the additional requirement of very fast simulation.

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http://dx.doi.org/10.1016/j.camwa.2014.02.006
0898-1221/

There is not much mathematical literature on the modeling of gas dynamics in an exhaust pipe in the literature. We mention [1–3] on studies regarding the temperature in the converter based on more complex chemical models, with assumed homogeneous gas dynamics. Furthermore, we mention fully compressible fluid dynamic models for the exhaust tube, where the aim is not primarily the determination of the converter temperature but the computation of sound waves (see, e.g., [4,5]) or mechanical properties of the exhaust tube (see, e.g., [6,7]).

A model which promises to be appropriate was developed recently in [8,9]. We shortly summarize the main features of this model:

- The model is one dimensional in space. The spacial axis is along the exhaust tube and all the values are mean values over the (non constant) cross sections.
- The basis is a fully compressible multi component gas dynamic model including surface friction and heat transfer through the surface, i.e., the exhaust tube walls.
- In this application the flow velocities are small (compared to the speed of sound), i.e., the Mach number is small. This fact is used to build a small Mach number asymptotic model in order to rule out sound waves. This reduces the simulation times significantly.
- We use two gas components to model the underlying complex chemistry, namely burnt and unburnt gas. However, the crucial quantity for the heating in the catalytic converters is the total heat release of the chemical reaction which can easily be included in such a simple two component reaction model.
- The exhaust tube is modeled as a network of tubes with constant cross section.

Neither for the pre-asymptotic hyperbolic model – a system of nonlinear hyperbolic balance laws – nor for the asymptotic (hyperbolic–elliptic-like) model a well-posedness theory is available. This is a common problem in many complex, multi-physics, systems. However, assuming existence of a unique solution and differentiability with respect to the inflow of unburnt gas, we will derive a system of differential equations yielding the continuous adjoint to the calculated flow. These will be used to find an optimal inflow profile using a projected gradient method.

We remark that, even in the pre-asymptotic regime, i.e., for hyperbolic systems – and even for scalar nonlinear hyperbolic equations – questions of uniqueness, differentiability, and optimality conditions are a field of active research. To give an impression of the different questions under consideration see, e.g., [10] for well-posedness of hyperbolic problems on networks, [11] for sensitivity analysis of hyperbolic conservation laws, [12,13] for optimization problems with hyperbolic equations on networks, [14] for control of Burgers equation with vanishing viscosity, or [15] for the control of unsteady compressible fluids.

The asymptotic model, under consideration, allows direct simulations almost in real time on a standard laptop computer. The model derived in [8] was built on the basis of models proposed in [16,17]. In order to validate the accuracy of the asymptotic model, we compared its numerical solutions to the ones of the fully hyperbolic problem and found a good agreement (see [8]).

Although it seems that we have drastically reduced the complexity of the model both from the application and mathematical point of view, we keep an appropriate, valid, and highly complex problem. From the application point of view, we deal with compressible low Mach number gas dynamics. Such problems arise in many application; ranging from astrophysics, meteorology to many engineering applications, e.g., gas pipeline networks [18]. From the mathematical point of view, we still have a multi component nonlinear system of PDE's on a network. To do optimization on such a model is still a highly challenging topic. We mention only a few papers where similarly complex issues where studies. In [19] optimization of non reactive gas flow in a pipeline is considered, whereas the optimal control for traffic flow is discussed in [12]. In [20] the optimal control of glass cooling is studied.

The paper is organized as follows. In Section 2, we introduce the model, whose main parts were derived in [8]. In Section 3, we define the optimization problem. In Section 4, we derive the optimality system. Section 5 is devoted to the discretization. Finally, in Section 6, we present numerical examples.

2. Model

The following dimensionless model describes the gas dynamics in an exhaust pipe.

$$\begin{aligned}
(A\rho)_t + (A\rho u)_x &= 0, \\
(A\rho u)_t + (A\rho u^2)_x + \frac{1}{\varepsilon} A p_x &= -C_f \rho \frac{u|u|}{2} - C_c A \chi \rho u, \\
\left(A\rho T + \varepsilon \frac{R}{c_v} A\rho \frac{u^2}{2}\right)_t + \left(A\rho u T + \varepsilon \frac{R}{c_v} A\rho \frac{u^3}{2} + \frac{R}{c_v} A u p\right)_x &= -h(T - T_{\text{Wall}}) + q_0 A \chi \rho z K(T), \\
(A\rho z)_t + (A\rho u z)_x &= -A\chi \rho z K(T), \\
p &= \rho T,
\end{aligned} \tag{1}$$

with the unknowns ρ, u, p, T, z as density, velocity, pressure, temperature, and ratio of unburnt gas, respectively. The terms on the left hand side originate from the one-dimensional Euler equations of gas dynamic in a pipe with variable cross section